

Supporting Information for

***Pendant Hydrogen-bond Donors in Cobalt Catalysts
Independently Enhance CO₂ Reduction***

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General

All manipulations of air and moisture sensitive materials were conducted under a nitrogen atmosphere in a Vacuum Atmospheres drybox or on a dual manifold Schlenk line. The glassware was oven-dried prior to use. All solvents were degassed with nitrogen and passed through activated alumina columns and stored over 4Å Linde-type molecular sieves. Deuterated solvents were dried over 4Å Linde-type molecular sieves prior to use. Proton NMR spectra were acquired at room temperature using Varian (Mercury 400 2-Channel, VNMRS-500 2-Channel, VNMRS- 600 3-Channel, and 400-MR 2-Channel) spectrometers and referenced to the residual ^1H resonances of the deuterated solvent (^1H : CDCl_3 , δ 7.26; C_6D_6 , δ 7.16; CD_2Cl_2 , δ 5.32; CD_3CN , δ 2.94) and are reported as parts per million relative to tetramethylsilane. Elemental analyses were performed using Thermo Scientific™ FLASH 2000 CHNS/O Analyzers. All the chemical reagents were purchased from commercial vendors and used without further purification. The ligands **L**¹⁻⁶ and complexes **1**^(II) and **6**^(II) were prepared according to the reported literature procedures^{1, 2}.

Cyclic Voltammetry (CV)

Electrochemistry experiments were carried out using a Pine potentiostat. The experiments were performed in a single compartment electrochemical cell under nitrogen or CO_2 atmosphere using a 3 mm diameter glassy carbon electrode as the working electrode, a platinum wire as auxiliary electrode and a silver wire as the reference electrode. Ohmic drop was compensated using the positive feedback compensation implemented in the instrument. All experiments in this paper were referenced relative to ferrocene (Fc) with the $\text{Fe}^{3+/2+}$ couple at 0.0 V. Alternatively, in cases when the redox couple of ferrocene overlapped with other redox waves of interest, decamethylferrocene (Fc^*) was used as an internal standard with the $\text{Fe}^{*3+/2+}$ couple at -0.48 V. All electrochemical experiments were performed with 0.1 M tetrabutylammonium hexafluorophosphate as supporting electrolyte. The concentrations of the cobalt complexes **1**^(II)–**6**^(II) were generally at 0.5 mM and experiments with CO_2 were performed at gas saturation or varying amounts of CO_2 in dimethylformamide (DMF).

Controlled-potential electrolysis (CPE)

CPE measurements were conducted in a two-chambered H cell. The first chamber held the working and reference electrodes in 50 mL of 0.1 M tetrabutylammonium hexafluorophosphate and 0.5 M methanol in DMF. The second chamber held the auxiliary electrode in 25 mL of 0.1 M tetrabutylammonium hexafluorophosphate in DMF. The two chambers were separated by a fine porosity glass frit. The reference electrode was placed in a separate compartment and connected by a Vycor tip. Glassy carbon plate electrodes (6 cm \times 1 cm \times 0.3 cm; Tokai Carbon USA) were used as the working and auxiliary electrodes. Using a gas-tight syringe, 10 mL of gas were withdrawn from the headspace of the H cell and injected into a gas chromatography instrument (Shimadzu GC-2010-Plus) equipped with a BID detector and a Restek ShinCarbon ST Micropacked column. Faradaic efficiencies were determined by diving

the measured CO produced by the amount of CO expected based on the charge passed during the bulk electrolysis experiment. For each species the controlled-potential electrolysis measurements were performed at least twice, leading to similar behavior. The reported Faradaic efficiencies and mmol of CO produced are average values.

TOF calculations from cyclic voltammetry³

Equations 1–5 were used to determine TOF from catalytic CVs. The catalytic current (i_{cat}) for an EECC process (E = electrochemical, C = chemical step) is given by eq 1, and it corresponds to the plateau current. This equation assumes a one-electron diffusion current and pseudo-first-order kinetics (the reaction is first order in catalyst and the concentrations of the substrates, Q (CO₂), is large in comparison to the concentration of catalyst). In eq 1, F is Faraday's constant ($F = 96\,485\text{ C/mol}$), S is the surface area of the electrode ($A = 0.07065\text{ cm}^2$ for CVs), C_{cat}^0 is the catalyst concentration ($[cat] = 0.5\text{ mM} = 5 \times 10^{-7}\text{ mol/cm}^3$), D_{cat} is the diffusion constant of the catalytically-active species ($\sim 5 \times 10^{-6}\text{ cm}^2/\text{s}$), and k_{cat} is the rate constant of the catalytic reaction.

$$i_{cat} = FSC_{cat}^0\sqrt{D_{cat}}\sqrt{2k_{cat}} \quad (1)$$

Equation 1 is simplified by standardizing with the current in the absence of substrate (CO₂ in this case), as described by eq 2. In eq 2, F is Faraday's constant ($F = 96\,485\text{ C/mol}$), S is the surface area of the electrode ($A = 0.07065\text{ cm}^2$ for CVs), C_{cat}^0 is the catalyst concentration ($[cat] = 0.5\text{ mM} = 5 \times 10^{-7}\text{ mol/cm}^3$), D_{cat} is the diffusion constant of the catalytically-active species ($\sim 5 \times 10^{-6}\text{ cm}^2/\text{s}$), v is the scan rate (0.1 V/s), R is the universal gas constant ($R = 8.31\text{ J K}^{-1}\text{ mol}^{-1}$), and T is temperature ($T = 298.15\text{ K}$).

$$i_p = 0.446 \times FSC_{cat}^0\sqrt{D_{cat}}\sqrt{\frac{Fv}{RT}} \quad (2)$$

Dividing eq 1 by eq 2 allows for determination of i_{cat}/i_p and allows one to further calculate the catalytic rate constant (k_{cat}) without having to determine S, C_{cat}^0 , and D_{cat} . The ratio of equations 1 and 2 produces equation 3 which can be rearranged to produce equation 4 in which k_{cat} can be solved directly.

$$\frac{i_{cat}}{i_p} = \frac{1}{0.446} \times \sqrt{\frac{2k_{cat}}{v} \frac{RT}{F}} = 2.24 \times \sqrt{\frac{2k_{cat}}{v} \frac{RT}{F}} \quad (3)$$

$$k_{cat} = \left(\frac{i_{cat}}{i_p}\right)^2 \frac{v}{2.24^2} \frac{F}{2RT} \quad (4)$$

Finally, eq 4 can be simplified into eq 5, from which k_{cat} can be calculated directly.

$$k_{cat} = 0.387 \times \left(\frac{i_{cat}}{i_p}\right)^2 \quad (5)$$

In the above calculations, the i_p values used correspond to the peak current obtained from the $\text{Co}^{\text{I/0}}$ reduction. However, given that the $\text{Co}^{\text{I/0}}$ reduction is quasi-reversible, its homogeneity cannot be tested. Therefore, we have also performed the plateau current analysis using i_p values obtained from the reversible (homogeneous) $\text{Co}^{\text{II/I}}$ couple and obtained identical results.

TOF_{CPE} calculations from controlled potential electrolysis³

Equation 6 was used to determine TOF from CPE data, as previously reported¹. This equation assumes that electron transfer to the catalyst is fast, obeying the Nernst law. In eq 6, i is the stable current transferred during CPE ($i = \text{charge} \times \text{F.E.}/\text{time}$, C/s), F is Faraday's constant ($F = 96485 \text{ C/mol}$), A is the surface area of the working electrode ($A = 3 \text{ cm}^2$ for CPE), k_{cat} is the overall rate constant of the catalytic reaction, D is the diffusion coefficient ($\sim 5 \times 10^{-6} \text{ cm}^2/\text{s}$), $[\text{cat}]$ is the concentration of the catalyst without substrate ($[\text{cat}] = 0.5 \text{ mM} = 5 \times 10^{-7} \text{ mol/cm}^3$), R is the universal gas constant ($R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$), T is temperature ($T = 298.15 \text{ K}$), $F/RT = 38.92 \text{ V}^{-1}$. When the electrolysis potential is on the plateau of the catalytic wave, the following eq can be used to calculate TOF, as previously reported³.

$$TOF = k_{\text{cat}} = \frac{i^2}{F^2 A^2 D [\text{cat}]^2} \quad (6)$$

Controlled potential electrolysis (CPE) experiments, on the other hand, are bulk experiments that are run for prolonged periods of time and under constant stirring, and therefore, replenishing of the catalyst in the diffusion layer (at the electrode-liquid interface). In these experiments, the rate is limited by catalyst, substrate, reagents and products (catalyst, CO_2 , TFE, CO) diffusion to and away from the electrode. These experiments provide information about the stability and selectivity of the catalyst, but do not provide any kinetic information intrinsic to the catalyst³.

Evan's Method⁴

Evan's method was used to determine the total spin (S) of a metal complex by ^1H NMR spectroscopy. Equation 7 is used to determine the MMs (Measured Molar Susceptibility). ΔHz is the difference in hertz between the peaks of the solvent in contact with the complex and the ones in the capillary tube and, M is the molarity of the sample (in units of mol/L), and Hz_{NMR} is the spectrometer frequency, in hertz (500,000,000).

$$MMs = \frac{3000 \times \Delta\text{Hz}}{4\pi \times M \times \text{Hz}_{\text{NMR}}} \quad (7)$$

- For $\mathbf{1}^{\text{(II)}}$, $\Delta\text{Hz} = 90.5 \text{ Hz}$
- For $\mathbf{1}^{\text{(I)}}$, $\Delta\text{Hz} = 131.5 \text{ Hz}$

Subsequently, eqs 8 and 9 are used to determine the number of unpaired electrons

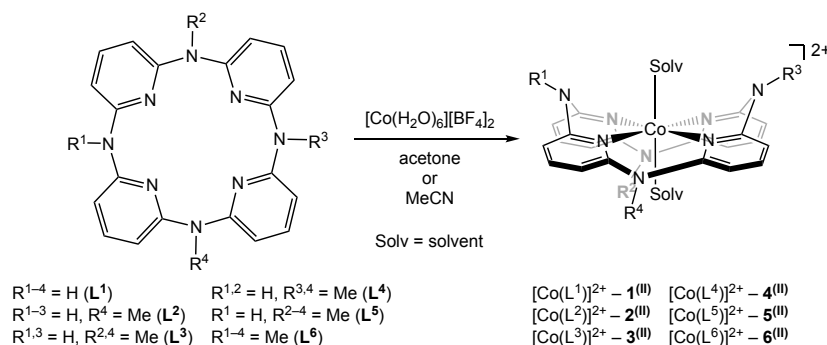
$$X_p = MMs - X_D, \quad X_D = \frac{mM}{2} \times 10^{-6} \quad (8)$$

$$\mu_{eff} = 2.84\sqrt{T \times X_P} \quad (9)$$

X_P corresponds to the corrected molar susceptibility, mM is the molar mass of the sample (in units of g/mol), and T is the temperature in Kelvin (293 K)

- For **1^(III)** $mM = 720 \text{ g/mol}$
- For **1^(I)**, $mM = 513 \text{ g/mol}$
- The value obtained for μ_{eff} :
 - **1^(III)** is: 3.63 Bohr Magnetons. **Three unpaired** electrons correspond to an expected value of 3.87
 - **1^(I)** is: 2.92 Bohr Magnetons. **Two unpaired** electrons correspond to an expected value of 2.83

Synthesis



[CoL²][BF₄]₂ (2^(III)). [Co(MeCN)₆][BF₄]₂ (27.1 mg, 0.070 mmol) in acetone (1 mL) was added to a solution of **L²** (16.7 mg, 0.071 mmol) in acetone (2 mL) giving rise to a brown solution. The mixture was allowed to stir for 5 minutes. The solution was filtered through a microfiber filter. Slow diffusion with diethyl ether produced orange crystals in quantitative yields. ¹H NMR (400 Hz, MeCN-*d*₃) δ 19.19–18.34 (m, 8H, *m*-NC₅H₃), 12.06–11.72 (m, 4H, *p*-NC₅H₃), 10.99 (s, 1H, NH), 8.40 (s, 2H, NH), 2.445 (s, 3H, CMe). Anal. calcd for [Co(L²)][BF₄]₂·(Et₂O)·(Cl₂CH₂)·(NCCH₃) (C₂₈H₃₃B₂Cl₂CoF₈N₉O): C, 41.26 H, 4.96; N, 15.47. Found: C, 41.30; H, 3.53; N, 15.00.

[CoL³][BF₄]₂ (3^(III)). [Co(MeCN)₆][BF₄]₂ (35.0 mg, 0.088 mmol) in acetone (1 mL) was added to a solution of **L³** (20.5 mg, 0.088 mmol) in acetone (2 mL) giving rise to a brown solution. The mixture was allowed to stir for 5 minutes. The solution was filtered through a microfiber filter. Slow diffusion with diethyl ether produced orange crystals in quantitative yields. ¹H NMR (400 Hz, MeCN-*d*₃) δ 10.80 (s, 2H), 10.33 (s, 2H), 6.57 (s, 4H), 3.56–5.13 (m, 10H), 2.81 (s, 4H). Anal. calcd for [Co(L³)][BF₄]₂·(acetone)₂·(H₂O)₂ (C₂₈H₃₆B₂CoF₈N₈O₄): C, 43.05; H, 4.65; N, 14.34. Found: C, 43.55; H, 4.08; N, 14.28.

[CoL⁴][BF₄]₂ (4^{II}). [Co(MeCN)₆][BF₄]₂ (29.4 mg, 0.074 mmol) in acetone (1 mL) was added to a solution of **L⁴** (18 mg, 0.077 mmol) in acetone (2 mL) giving rise to a brown solution. The mixture was allowed to stir for 5 minutes. The solution was filtered through a microfiber filter. Slow diffusion with diethyl ether produced orange crystals in quantitative yields. ¹H NMR (400 Hz, MeCN-*d*₃) δ 12.92 (s, 2H), 11.21–10.24 (m, 5H), 8.81 (d, 4H), 7.75 (s, 6H), 4.86 (s, 2H). Anal. calcd for [Co(L⁴)]₂·(Et₂O)·(H₂O)₂ (C₂₆H₃₄B₂CoF₈N₈O₃): C, 42.25; H, 4.64; N, 15.16. Found: C, 42.17; H, 4.01; N, 14.75.

[CoL⁵][BF₄]₂ (5^{II}). [Co(MeCN)₆][BF₄]₂ (26.6 mg, 0.065 mmol) in acetone (1 mL) was added to a solution of **L⁵** (15.2 mg, 0.065 mmol) in acetone (2 mL) giving rise to a brown solution. The mixture was allowed to stir for 5 minutes. The solution was filtered through a microfiber filter. Slow diffusion with diethyl ether produced orange crystals in quantitative yields. ¹H NMR (400 Hz, MeCN-*d*₃) δ 12.24 (s, 1H), 10.89 (s, 4H), 9.38 (s, 4H), 8.18 (s, 4H), 3.30 (s, 8H). Anal. calcd for [Co(L⁵)]₂·(Et₂O)·(H₂O)₂ (C₂₃H₂₂B₂CoF₈N₈): C, 42.96; H, 3.45; N, 17.43. Found: C, 42.64; H, 3.60; N, 17.53.

Crystallographic data

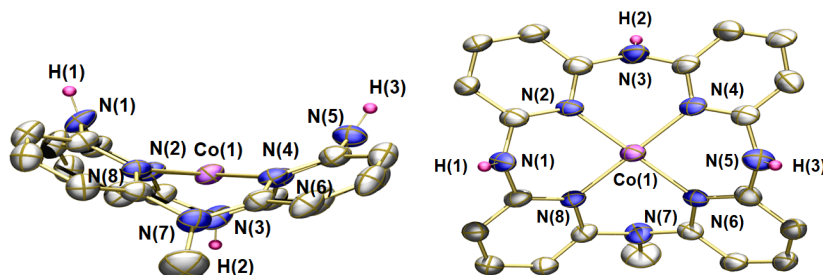


Figure S1. Side (left) and top (right) views of the solid state structure of **2^{II}**. Hydrogen atoms, non-coordinating anions, and solvent molecules are omitted for clarity.

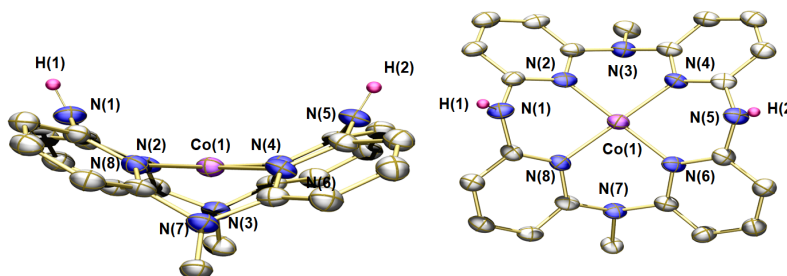


Figure S2. Side (left) and top (right) views of the solid state structure of **3^{II}**. Hydrogen atoms, non-coordinating anions, and solvent molecules are omitted for clarity.

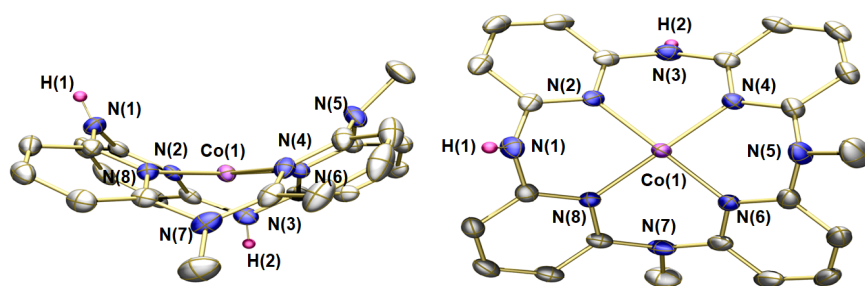


Figure S3. Side (left) and top (right) views of the solid state structure of 4^(II). Hydrogen atoms, non-coordinating anions, and solvent molecules are omitted for clarity.

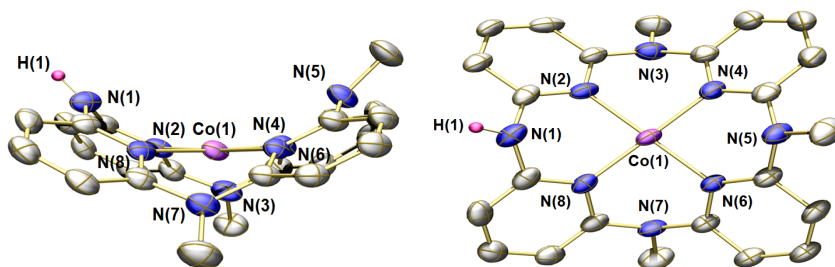


Figure S4. Side (left) and top (right) views of the solid state structure of 5^(II). Hydrogen atoms, non-coordinating anions, and solvent molecules are omitted for clarity.

Table S1. Crystal data and structure refinement for **2^(II)**.

Identification code	Alon092616	
Chemical formula	C ₂₅ H ₂₄ B ₂ CoF ₈ N ₁₀	
Formula weight	697.09 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.020 × 0.140 × 0.180 mm	
Crystal habit	clear pale orange blade	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 12.026(6)$ Å	$\alpha = 72.461(8)^\circ$
	$b = 12.302(6)$ Å	$\beta = 79.742(8)^\circ$
	$c = 14.145(7)$ Å	$\gamma = 64.354(8)^\circ$
Volume	1796.0(15) Å ³	
Z	2	
Density (calculated)	1.289 g/cm ³	
Absorption coefficient	0.549 mm ⁻¹	
F(000)	706	
Diffractionmeter	Bruker APEX DUO	
Radiation source	fine-focus tube, MoK α	
Theta range for data collection	1.88 to 24.71°	
Index ranges	$-14 \leq h \leq 14, -14 \leq k \leq 14, -16 \leq l \leq 16$	
Reflections collected	30085	
Independent reflections	6104 [R(int) = 0.0928]	
Coverage of independent reflections	99.6%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9890 and 0.9080	
Structure solution technique	direct methods	
Structure solution program	SHELXTL XT 2014/4 (Bruker AXS, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXTL XL 2014/7 (Bruker AXS, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6104 / 480 / 444	
Goodness-of-fit on F^2	1.046	
Final R indices	3971 data; $I > 2\sigma(I)$	$R_1 = 0.0868, wR_2 = 0.2252$
	all data	$R_1 = 0.1264, wR_2 = 0.2609$
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.1322P)^2 + 5.3242P]$ where $P = (F_o^2 + 2F_c^2)/3$	
Largest diff. peak and hole	1.038 and -0.678 eÅ ⁻³	
R.M.S. deviation from mean	0.102 eÅ ⁻³	

Table S2. Crystal data and structure refinement for **3^(II)**.

Identification code	Alon082916	
Chemical formula	C ₂₅ H ₃₀ B ₂ CoF ₈ N ₈ O ₃	
Formula weight	723.12 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal size	0.040 × 0.070 × 0.090 mm	
Crystal habit	clear light orange-brown prism	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 11.1267(14)$ Å	$\alpha = 106.688(8)^\circ$
	$b = 11.9052(15)$ Å	$\beta = 101.505(8)^\circ$
	$c = 12.2051(16)$ Å	$\gamma = 100.107(8)^\circ$
Volume	1470.1(3) Å ³	
Z	2	
Density (calculated)	1.634 g/cm ³	
Absorption coefficient	5.446 mm ⁻¹	
F(000)	738	
Diffractionmeter	Bruker APEX DUO	
Radiation source	IuS microsource, CuK α	
Theta range for data collection	3.92 to 68.22°	
Index ranges	$-13 \leq h \leq 13, -14 \leq k \leq 14, -14 \leq l \leq 14$	
Reflections collected	29257	
Independent reflections	5297 [R(int) = 0.1232]	
Coverage of independent reflections	98.4%	
Absorption correction	multi-scan	
Max. and min. transmission	0.8120 and 0.6400	
Structure solution technique	direct methods	
Structure solution program	SHELXTL XT 2014/5 (Bruker AXS, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXTL XL 2014/7 (Bruker AXS, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5297 / 502 / 449	
Goodness-of-fit on F^2	1.005	
Δ/σ_{\max}	0.005	
Final R indices	2323 data; $I > 2\sigma(I)$	$R_1 = 0.0894, wR_2 = 0.2097$
	all data	$R_1 = 0.2020, wR_2 = 0.2724$
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.1518P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	
Largest diff. peak and hole	1.270 and -1.364 eÅ ⁻³	
R.M.S. deviation from mean	0.172 eÅ ⁻³	

Table S3. Crystal data and structure refinement for **4^(II)**.

Identification code	Alon92116	
Chemical formula	C ₂₄ H ₂₃ B ₂ CoF ₈ N ₉	
Formula weight	670.06 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.126 × 0.312 × 0.495 mm	
Crystal habit	clear orange prism	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 10.090(5)$ Å	$\alpha = 83.756(6)^\circ$
	$b = 11.516(5)$ Å	$\beta = 87.480(6)^\circ$
	$c = 12.743(6)$ Å	$\gamma = 77.894(6)^\circ$
Volume	1438.8(11) Å ³	
Z	2	
Density (calculated)	1.547 g/cm ³	
Absorption coefficient	0.681 mm ⁻¹	
F(000)	678	
Diffractometer	Bruker APEX DUO	
Radiation source	fine-focus tube, MoK α	
Theta range for data collection	1.61 to 27.48°	
Index ranges	$-13 \leq h \leq 13, -14 \leq k \leq 14, -16 \leq l \leq 16$	
Reflections collected	29017	
Independent reflections	6601 [R(int) = 0.0286]	
Coverage of independent reflections	100.0%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9190 and 0.7290	
Structure solution technique	direct methods	
Structure solution program	SHELXTL XT 2014/5 (Bruker AXS, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXTL XL 2014/7 (Bruker AXS, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6601 / 110 / 434	
Goodness-of-fit on F^2	1.035	
Δ/σ_{\max}	0.001	
Final R indices	5643 data; $I > 2\sigma(I)$	$R_1 = 0.0563, wR_2 = 0.1545$
	all data	$R_1 = 0.0664, wR_2 = 0.1636$
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0887P)^2 + 2.8248P]$ where $P = (F_o^2 + 2F_c^2)/3$	
Largest diff. peak and hole	1.442 and -0.613 eÅ ⁻³	
R.M.S. deviation from mean	0.093 eÅ ⁻³	

Table S4. Crystal data and structure refinement for **5^(II)**.

Identification code	Alon091216	
Chemical formula	C ₂₆ H ₂₈ B ₂ CoF ₈ N ₈ O	
Formula weight	701.11 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal size	0.040 × 0.080 × 0.120 mm	
Crystal habit	clear light orange prism	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 10.1224(7)$ Å	$\alpha = 84.499(5)^\circ$
	$b = 11.5342(8)$ Å	$\beta = 89.722(5)^\circ$
	$c = 12.3686(8)$ Å	$\gamma = 77.529(5)^\circ$
Volume	1403.33(17) Å ³	
Z	2	
Density (calculated)	1.659 g/cm ³	
Absorption coefficient	5.631 mm ⁻¹	
F(000)	714	
Diffractometer	Bruker APEX DUO	
Radiation source	IuS microsource, CuK α	
Theta range for data collection	3.59 to 68.32°	
Index ranges	$-12 \leq h \leq 12, -13 \leq k \leq 13, -14 \leq l \leq 14$	
Reflections collected	31703	
Independent reflections	5006 [R(int) = 0.0695]	
Coverage of independent reflections	97.3%	
Absorption correction	multi-scan	
Structure solution technique	direct methods	
Structure solution program	SHELXTL XT 2014/4 (Bruker AXS, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5006 / 13 / 449	
Goodness-of-fit on F^2	1.043	
Δ/σ_{\max}	0.015	
Final R indices	4058 data; $I > 2\sigma(I)$	$R_1 = 0.0698,$ $wR_2 = 0.1861$
	all data	$R_1 = 0.0858,$ $wR_2 = 0.1986$
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.1059P)^2 + 3.0075P]$ where $P = (F_o^2 + 2F_c^2)/3$	
Largest diff. peak and hole	1.055 and -0.801 eÅ ⁻³	
R.M.S. deviation from mean	0.085 eÅ ⁻³	

Electrochemical characterization

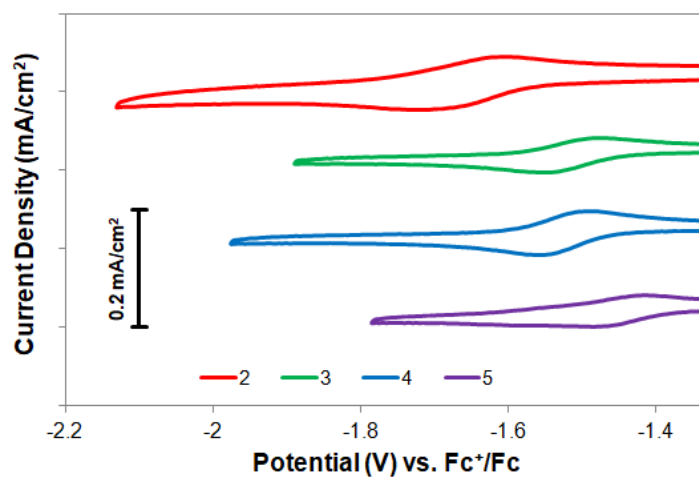


Figure S5. Cyclic voltammograms of complexes **2–5** (0.5 mM) in 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ in DMF under N_2 showcasing the reversible $\text{CoL}^{2+/+}$ couple.

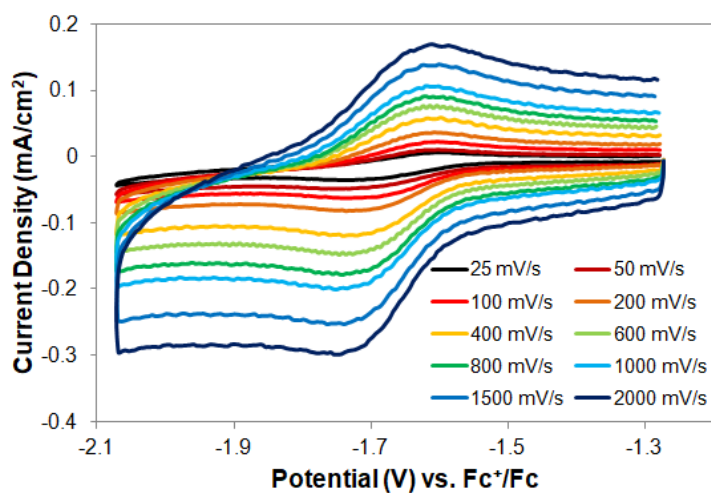


Figure S6. Cyclic voltammograms of 0.5 mM (**1**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the reversible one-electron reduction with an $E_{1/2}$ of -1.59 V vs. $\text{Fc}^{+/0}$ and assigned to $[\text{Co}(\text{L}^1)]^{2+/+}$ couple. Scan rates vary from 0.025 to 1 V/s.

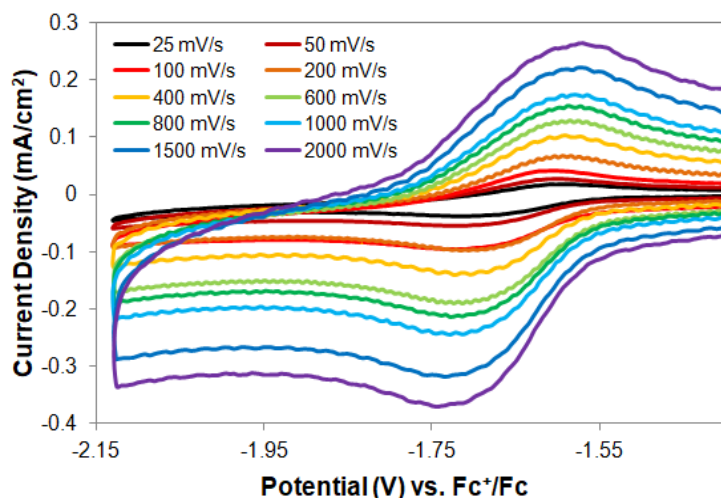


Figure S7. Cyclic voltammograms of 0.5 mM (**2**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the reversible one-electron reduction with an $E_{1/2}$ of $-1.66\text{ V vs. Fc}^{+/0}$ and assigned to $[\text{Co}(\text{L}^1)]^{2+/+}$ couple. Scan rates vary from 0.025 to 2 V/s.

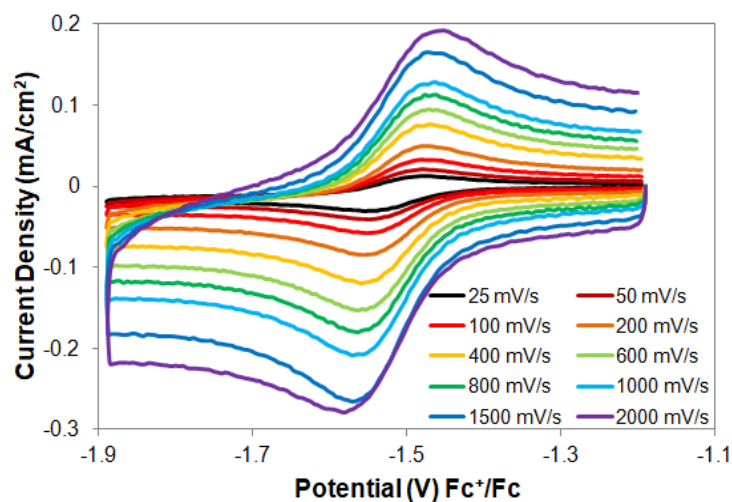


Figure S8. Cyclic voltammograms of 0.5 mM (**3**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the reversible one-electron reduction with an $E_{1/2}$ of $-1.53\text{ V vs. Fc}^{+/0}$ and assigned to $[\text{Co}(\text{L}^1)]^{2+/+}$ couple. Scan rates vary from 0.025 to 2 V/s.

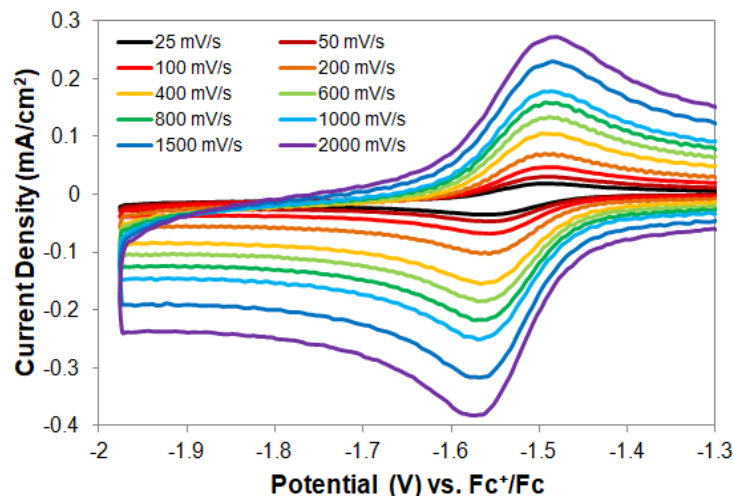


Figure S9. Cyclic voltammograms of 0.5 mM (**4**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the reversible one-electron reduction with an $E_{1/2}$ of -1.52 V vs. $\text{Fc}^{+/0}$ and assigned to $[\text{Co}(\text{L}^1)]^{2+/+}$ couple. Scan rates vary from 0.025 to 2 V/s.

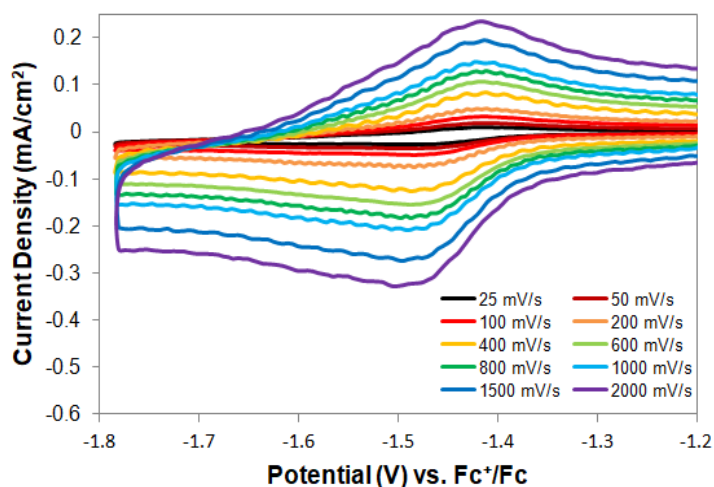


Figure S10. Cyclic voltammograms of 0.5 mM (**5**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the reversible one-electron reduction with an $E_{1/2}$ of -1.44 V vs. $\text{Fc}^{+/0}$ and assigned to $[\text{Co}(\text{L}^1)]^{2+/+}$ couple. Scan rates vary from 0.025 to 2 V/s.

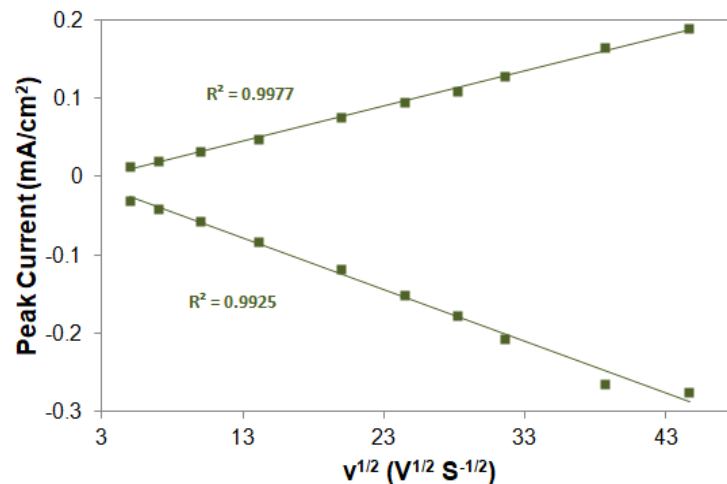


Figure S11. Plot showing that the peak current, both cathodic and anodic, in the cyclic voltammograms (CVs) of 0.5 mM (**2**) in a DMF solution containing 0.1 M [*n*Bu₄N][PF₆] under an atmosphere of N₂. The cathodic and anodic peak currents increase linearly with the square root of the scan rate. This behavior is indicative of a freely-diffusing species, where the electrode reaction is controlled by mass transport.

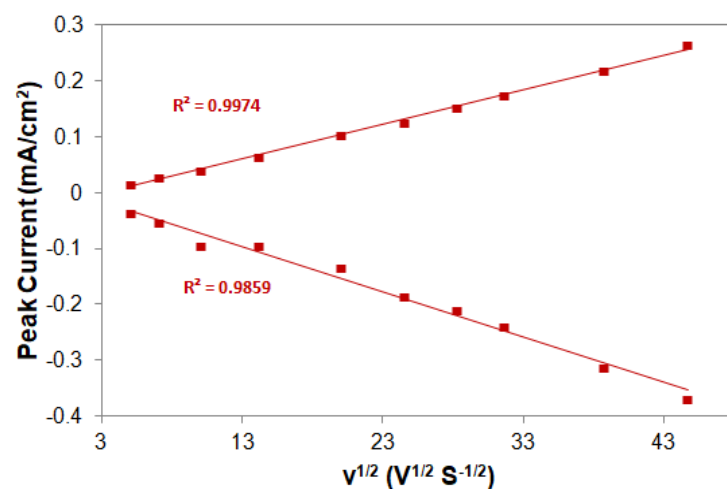


Figure S12. Plot showing that the peak current, both cathodic and anodic, in the cyclic voltammograms (CVs) of 0.5 mM (**3**) in a DMF solution containing 0.1 M [*n*Bu₄N][PF₆] under an atmosphere of N₂. The cathodic and anodic peak currents increase linearly with the square root of the scan rate. This behavior is indicative of a freely-diffusing species, where the electrode reaction is controlled by mass transport.

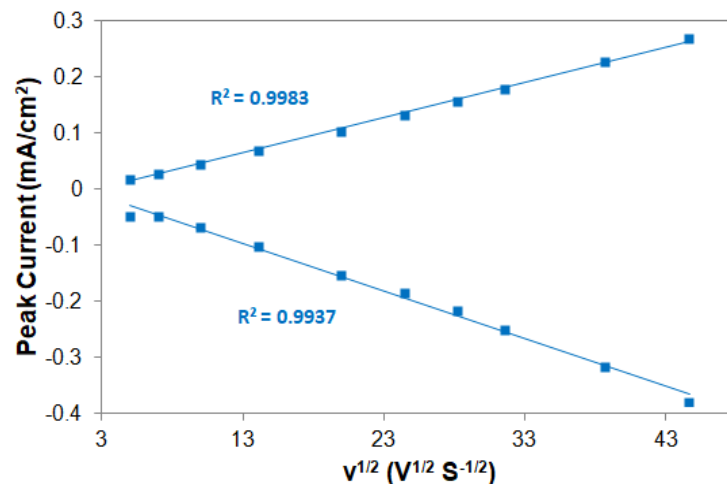


Figure S13. Plot showing that the peak current, both cathodic and anodic, in the cyclic voltammograms (CVs) of 0.5 mM (**4**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 . The cathodic and anodic peak currents increase linearly with the square root of the scan rate. This behavior is indicative of a freely-diffusing species, where the electrode reaction is controlled by mass transport.

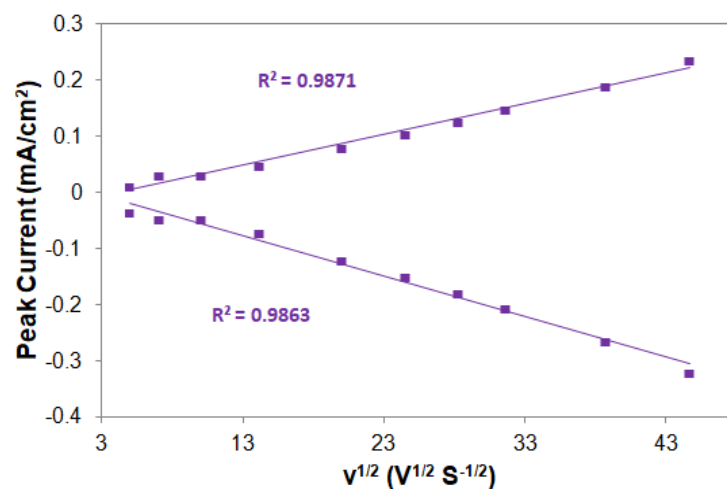


Figure S14. Plot showing that the peak current, both cathodic and anodic, in the cyclic voltammograms (CVs) of 0.5 mM (**5**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 . The cathodic and anodic peak currents increase linearly with the square root of the scan rate. This behavior is indicative of a freely-diffusing species, where the electrode reaction is controlled by mass transport.

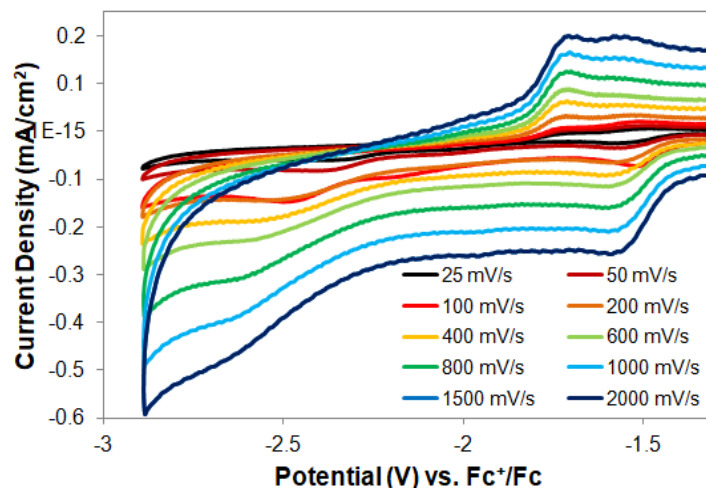


Figure S15. Cyclic voltammogram scan rate dependence of 0.5 mM (**1**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the $[\text{Co}(\text{L}^1)]^{2+/+}$ and $[\text{Co}(\text{L}^1)]^{+/0}$ couples. Scan rates vary from 0.025 to 2 V/s.

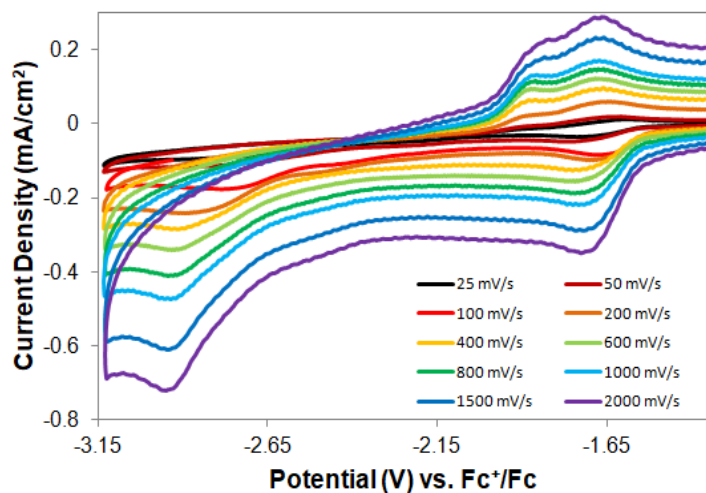


Figure S16. Cyclic voltammogram scan rate dependence of 0.5 mM (**2**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the $[\text{Co}(\text{L}^1)]^{2+/+}$ and $[\text{Co}(\text{L}^1)]^{+/0}$ couples. Scan rates vary from 0.025 to 2 V/s.

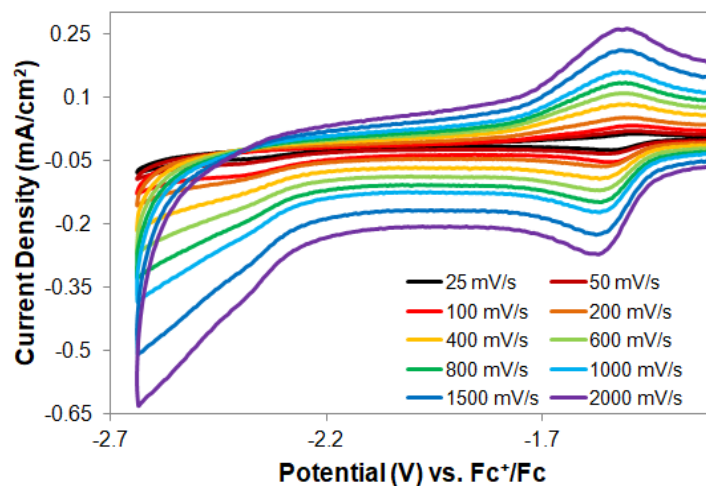


Figure S17. Cyclic voltammogram scan rate dependence of 0.5 mM (**3**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the $[\text{Co}(\text{L}^1)]^{2+/+}$ and $[\text{Co}(\text{L}^1)]^{+/0}$ couples. Scan rates vary from 0.025 to 2 V/s.

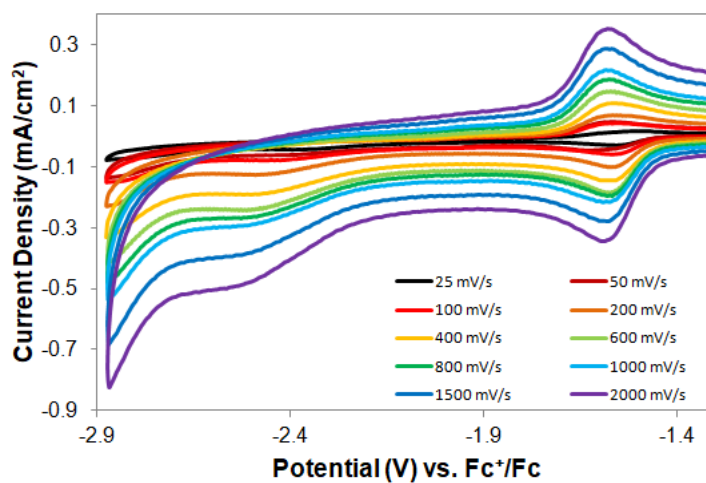


Figure S18. Cyclic voltammogram scan rate dependence of 0.5 mM (**4**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the $[\text{Co}(\text{L}^1)]^{2+/+}$ and $[\text{Co}(\text{L}^1)]^{+/0}$ couples. Scan rates vary from 0.025 to 2 V/s.

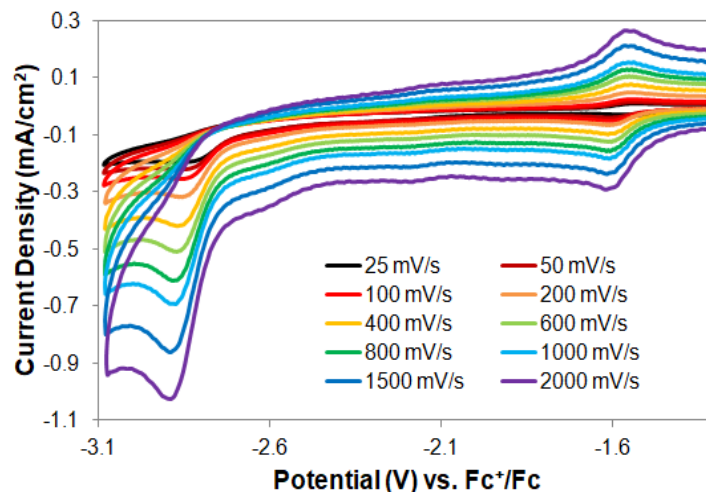


Figure S19. Cyclic voltammogram scan rate dependence of 0.5 mM (**5**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 displaying the $[\text{Co}(\text{L}^1)]^{2+/+}$ and $[\text{Co}(\text{L}^1)]^{+/0}$ couples. Scan rates vary from 0.025 to 2 V/s.

Mechanistic studies of CO_2 reduction catalysis

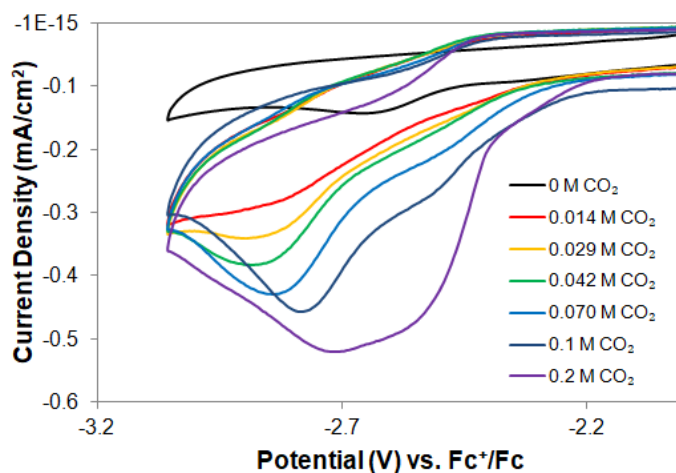


Figure S20. Linear scan voltammograms of **1** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 and in the presence of varying concentrations of CO_2 . Scan rates are 100 mV/s.

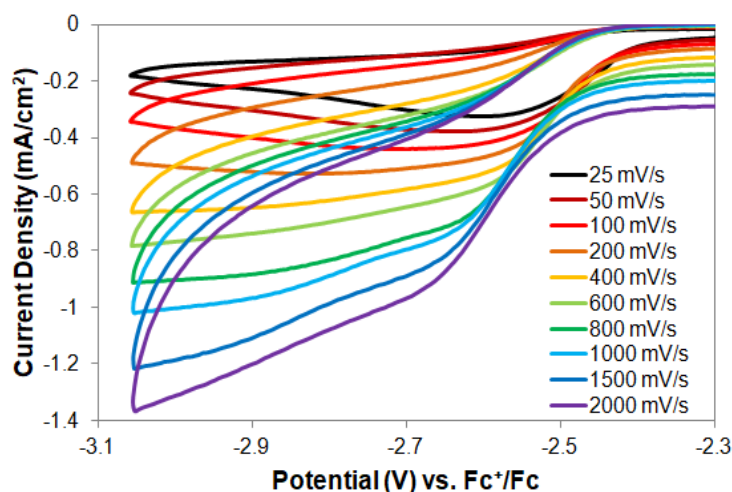


Figure S21. Cyclic voltammogram scan rate dependence of 0.5 mM (**1**) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of CO_2 . Scan rates vary from 0.025 to 2 V/s. This result is consistent with a fast interaction between CO_2 and cobalt complex.

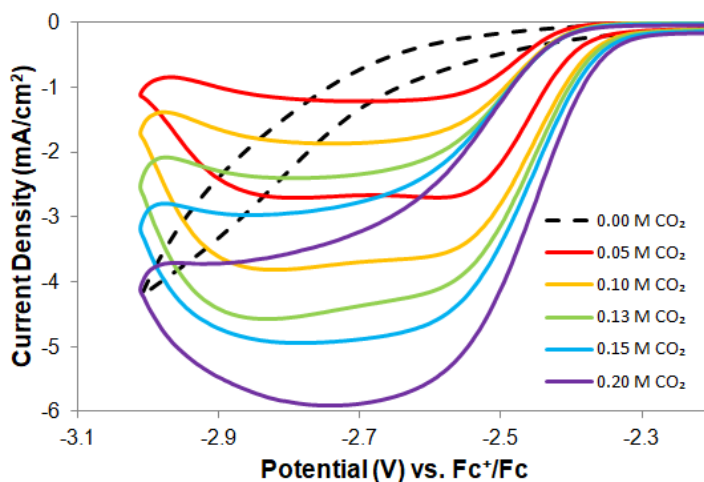


Figure S22. Linear scan voltammograms of **1** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$, TFE (1.2 M) and in the presence of varying $[\text{CO}_2]$. Scan rates are 100 mV/s.

Table S5. Rate constants at varying $[\text{CO}_2]$ at acid saturation conditions ($[\text{TFE}] = 1.2 \text{ M}$).

$[\text{CO}_2] \text{ (M)}$	$\frac{i_{cat}}{i_p}$	$k_{obs} \text{ (s}^{-1}\text{)}$
0.05	52.5	1,000
0.10	71.8	2,000
0.13	85.2	2,800
0.15	95.8	3,500
0.20	115.7	5,200

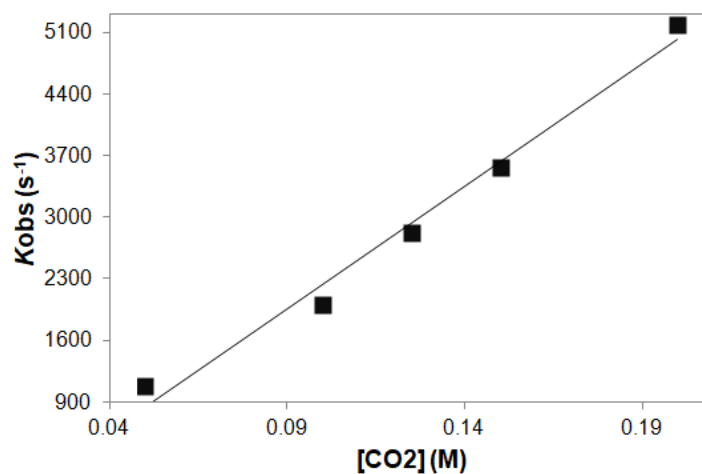


Figure S23. Plot of the observed rate constants k_{obs} vs. $[\text{CO}_2]$ in a DMF solution containing 0.1 M $[\text{nBu}_4\text{N}][\text{PF}_6]$, **1** (0.5 mM), and TFE (1.2 M). The linear relationship indicates that the reaction is first order with respect to CO_2 . The slope of the line corresponds to an overall rate constant of $27,800 \text{ M}^{-1}\text{s}^{-1}$.

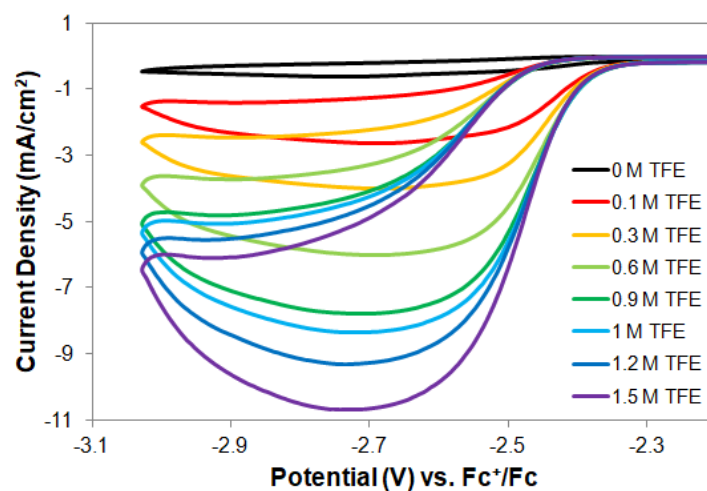


Figure S24. Linear scan voltammograms of **1** (0.5 mM) in a DMF solution containing 0.1 M $[\text{nBu}_4\text{N}][\text{PF}_6]$, CO_2 (0.20 M), and in the presence of varying $[\text{TFE}]$. Scan rates are 100 mV/s.

Table S6. Rate constants at varying [TFE] and at CO₂ saturation conditions ([CO₂] = 0.20 M).

[TFE] (M)	$\frac{i_{cat}}{i_p}$	$k_{obs} (s^{-1})$
0.1	51.5	1,000
0.3	78.6	2,400
0.6	117.6	5,300
0.9	152.3	8,900
1.0	163.9	10,400
1.2	181.8	12,800
1.5	208.8	16,900

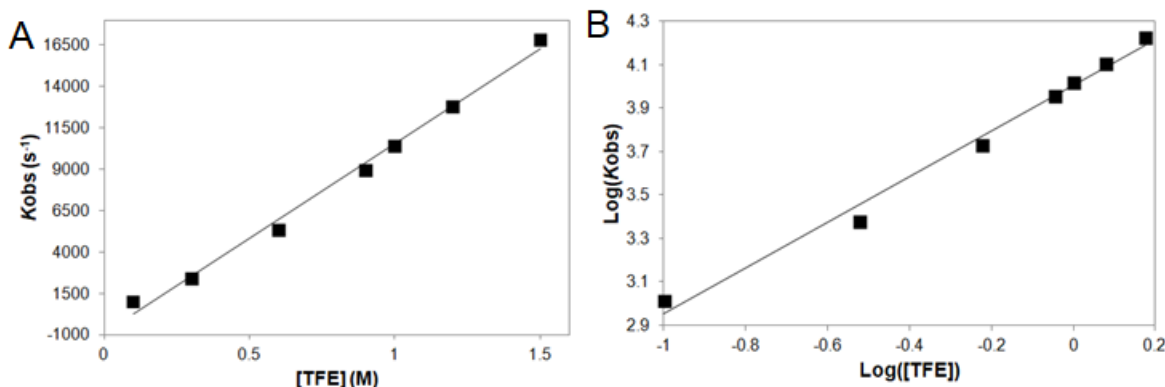


Figure S25. Linear (A) and Log-Log (B) plots of the observed rate constants k_{obs} vs. [TFE] in a DMF solution containing 0.1 M $[nBu_4N][PF_6]$, **1** (0.5 mM), and CO₂ (0.20 M). The slope of the linear plot corresponds to an overall rate constant of 11,400 M⁻¹s⁻¹. The Slope of the Log-Log plot is equal to one, indicating a first order dependence on protons.

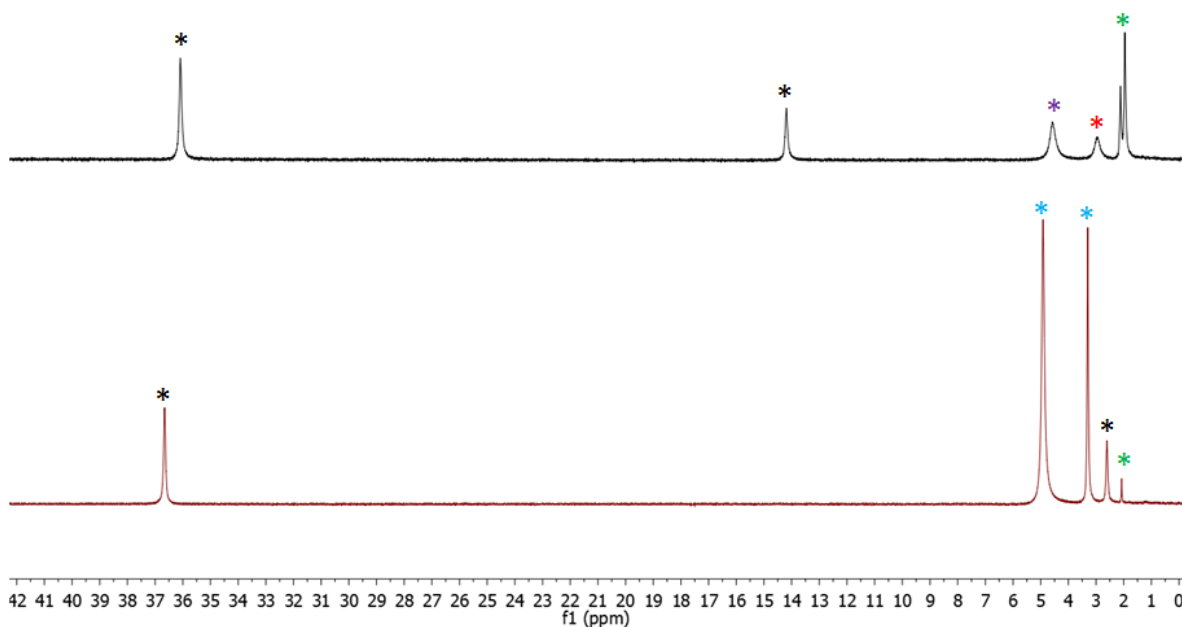


Figure S26. ^1H NMR spectra of **1** in acetonitrile- d_3 (top) and upon subsequent methanol- d_4 addition (bottom). Selected peaks correspond to: pyridine protons (*meta* and *para*) (black), acetonitrile (green), coordinated acetone (purple) and the amine NH protons (red), and residual methanol (blue).

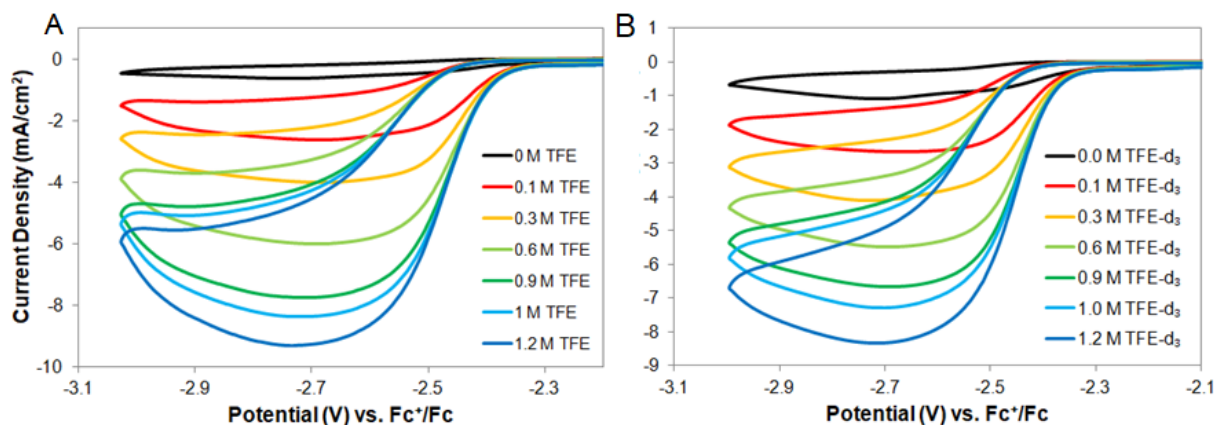


Figure S27. Linear scan voltammograms of **1** (0.5 mM) in a DMF solution containing 0.1 M $[\text{nBu}_4\text{N}][\text{PF}_6]$ under an atmosphere of CO_2 and in the presence of varying concentrations of TFE (A) and TFE- d_3 (B). Scan rates are 100 mV/s.

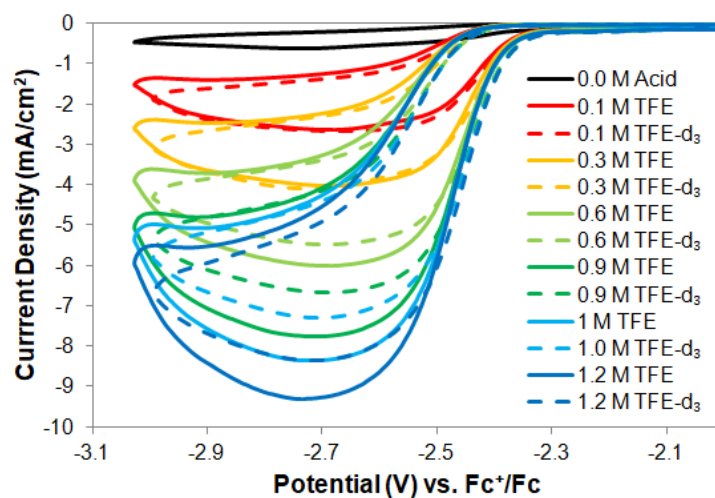


Figure S28. Linear scan voltammograms of **1** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of CO_2 and in the presence of varying concentrations of TFE (solid) and TFE-d_3 (dashed). Scan rates are 100 mV/s.

$[\text{TFE-d}_3]$ (M)	$\frac{i_{\text{cat}}}{i_p}$	k_{obs} (s^{-1})	$\text{KIE}_{\text{H/D}}$
0.1	51.4	1,000	1.0
0.3	78.8	2,400	1.0
0.6	106.0	4,300	1.2
0.9	128.5	6,400	1.4
1.0	140.8	7,700	1.3
1.2	160.8	10,011	1.3
1.5	172.0	11,500	1.5

Table S7. Rate constants at varying $[\text{TFE-d}_3]$ and at CO_2 saturation conditions ($[\text{CO}_2] = 0.20 \text{ M}$).

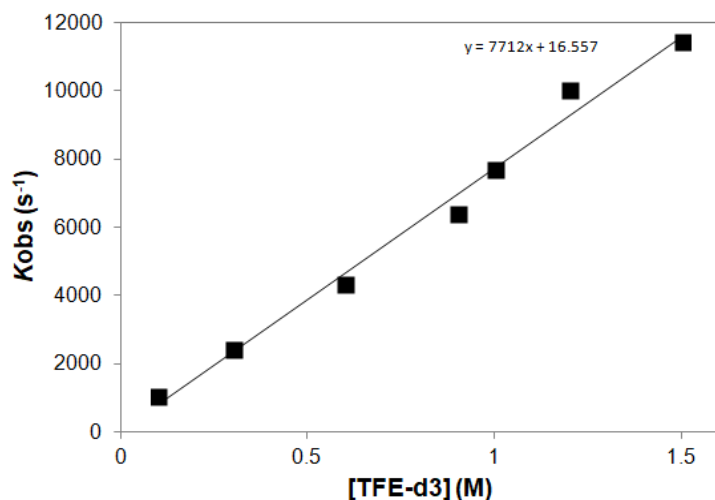


Figure S29. Plot of the observed rate constants k_{obs} vs. $[\text{TFE-}d_3]$ in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$, **1** (0.5 mM), and CO_2 (0.20 M). The linear relationship indicates that the reaction is first order with respect to $\text{TFE-}d_3$. The slope of the line corresponds to an overall rate constant of $7,700 \text{ M}^{-1}\text{s}^{-1}$.

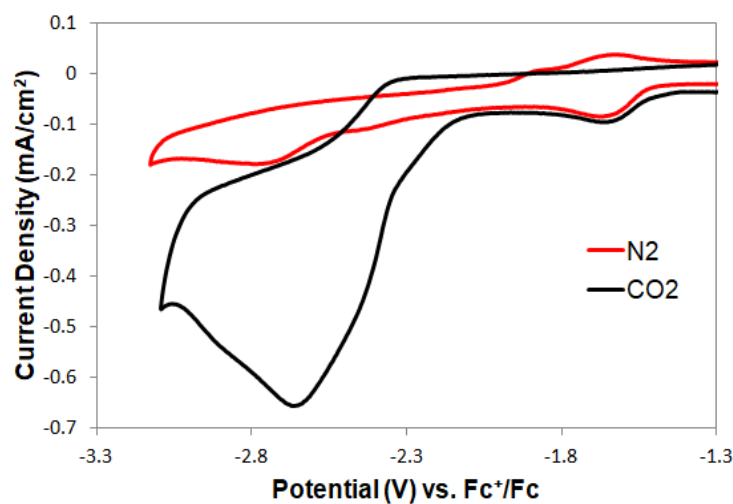


Figure S30. Cyclic voltammogram of 0.5 mM of **2** in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 (red) or CO_2 (black). Scan rate is 100 mV/s.

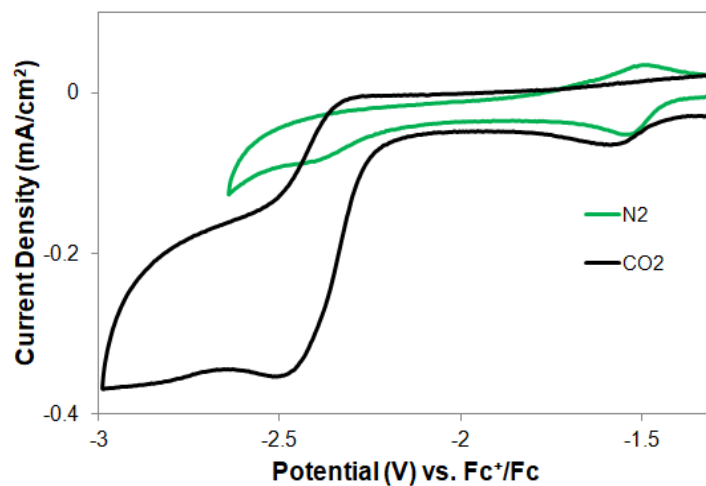


Figure S31. Cyclic voltammogram of 0.5 mM of **3** in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 (green) or CO_2 (black). Scan rate is 100 mV/s.

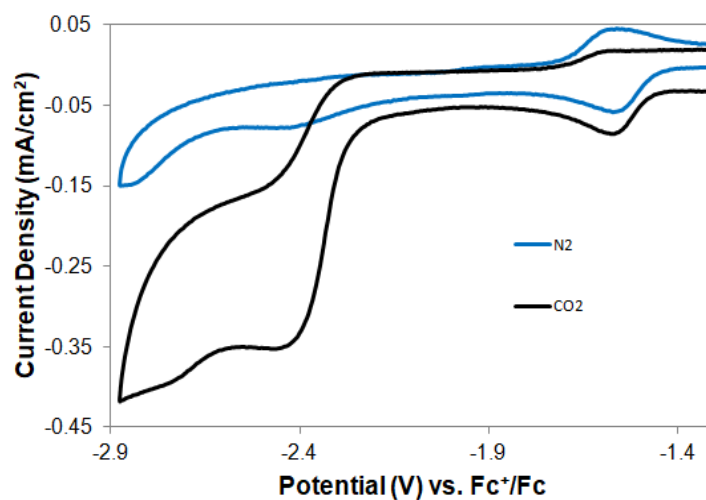


Figure S32. Cyclic voltammogram of 0.5 mM of **4** in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 (blue) or CO_2 (black). Scan rate is 100 mV/s.

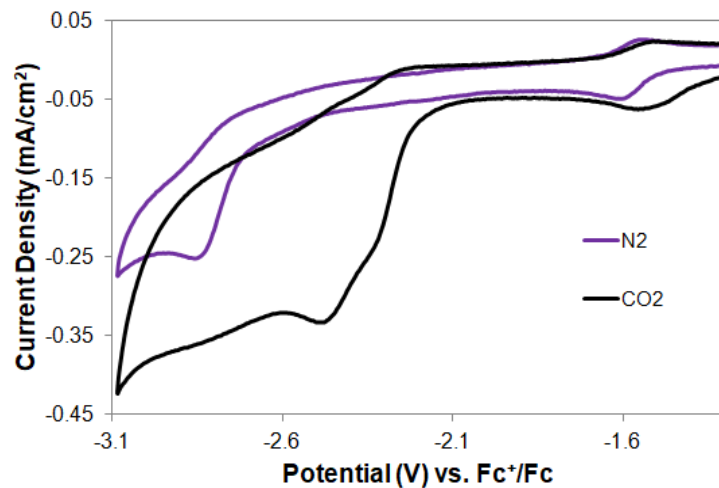


Figure S33. Cyclic voltammogram of 0.5 mM of **5** in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of N_2 (purple) or CO_2 (black). Scan rate is 100 mV/s.

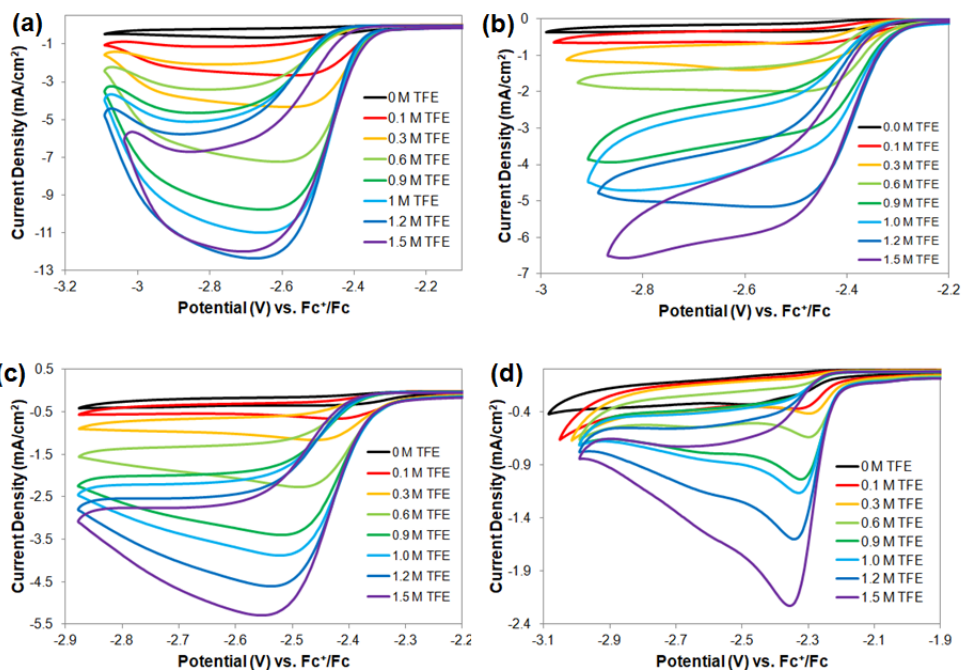


Figure S34. Titration curves for complexes **2–5** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$, and CO_2 (0.2 M), at 100 mV/s (a–d, respectively).

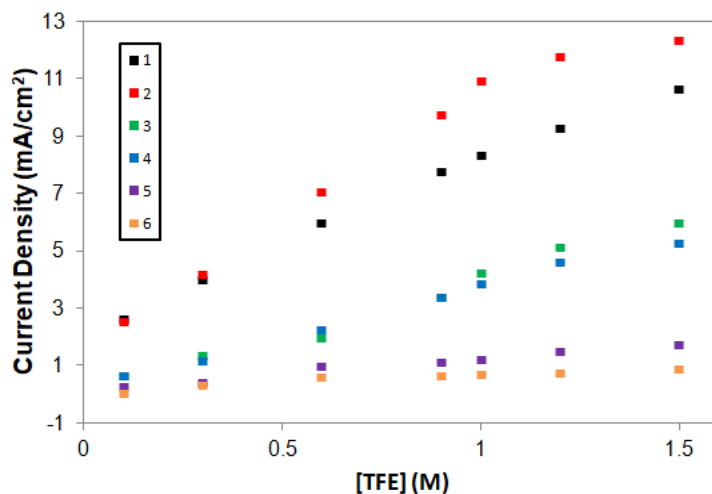


Figure S35. Plot of maximum current density versus the concentration of TFE for complexes **1–6** (0.5 mM) in 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ in DMF under CO_2 saturation (0.2 M). All scan rates are 100 mV/s.

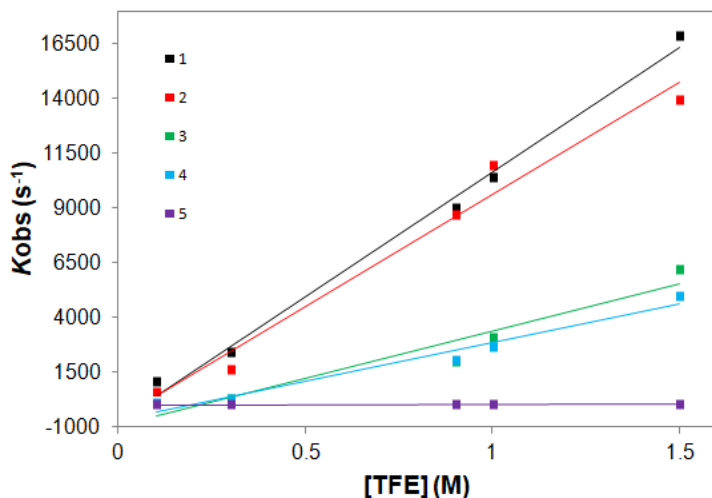


Figure S36. Plot of the observed rate constants k_{obs} vs. $[\text{TFE}]$ for complexes **1–5** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$, and CO_2 (0.2 M) at 100 mV/s. The linear relationship indicates that the reaction is first order with respect to TFE. The slopes of the lines correspond to the overall rate constant. The slopes are: 11,400, 10,257, 4,300, 3,600, 33, $\text{M}^{-1}\text{s}^{-1}$ for complexes **1–5**, respectively.

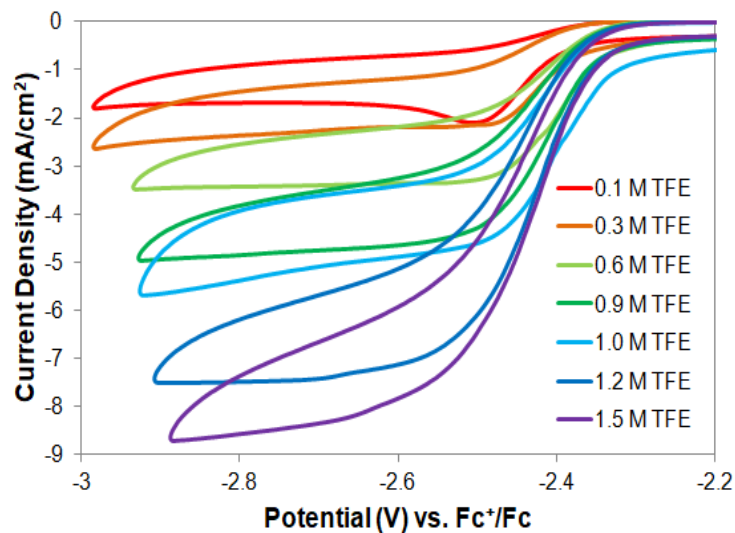


Figure S37. Linear scan voltammograms of **3** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of CO_2 and in the presence of varying concentrations of TFE. Scan rates are 2000 mV/s.

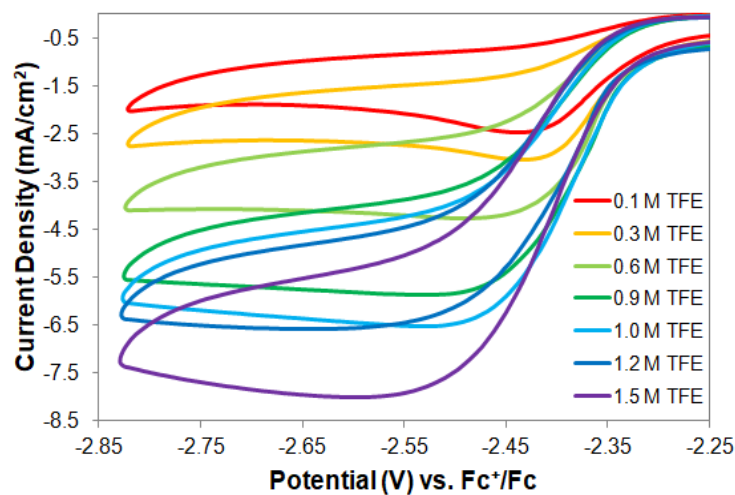


Figure S38. Linear scan voltammograms of **4** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of CO_2 and in the presence of varying concentrations of TFE. Scan rates are 2000 mV/s.

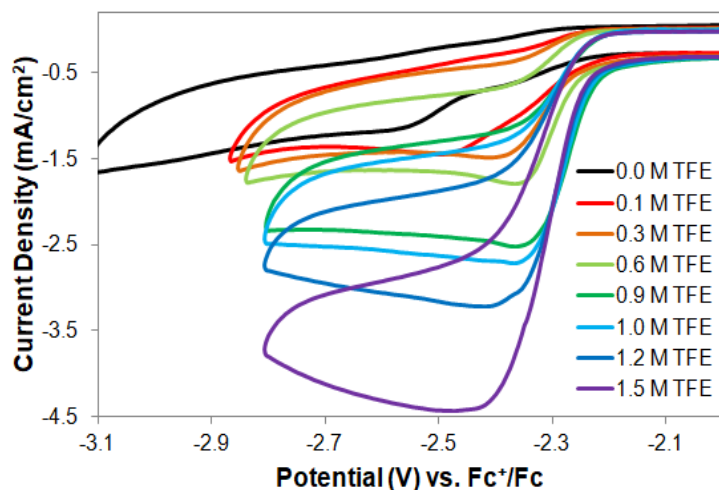


Figure S39. Linear scan voltammograms of **5** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of CO_2 and in the presence of varying concentrations of TFE. Scan rates are 2000 mV/s.

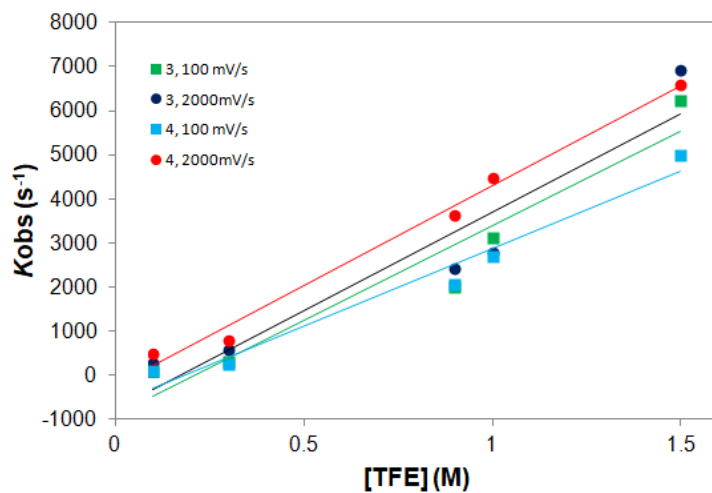


Figure S40. Plot of the observed rate constants k_{obs} vs. $[\text{TFE}]$ for complexes **3–4** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$, and CO_2 (0.2 M) at 100 mV/s and 2000 mV/s. The linear relationship and slope are scan rate independent at 4300 and 3600 for $\text{M}^{-1}\text{s}^{-1}$ for **3** and **4**, respectively

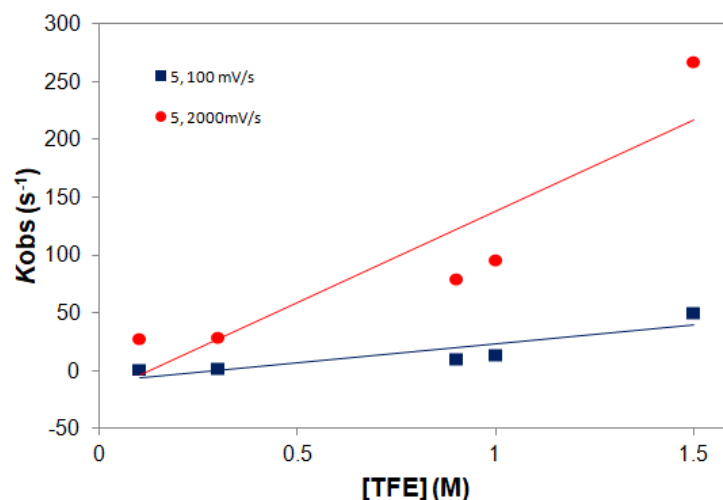


Figure S41. Plot of the observed rate constants k_{obs} vs. [TFE] for complex **5** (0.5 mM) in a DMF solution containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$, and CO_2 (0.2 M) at different scan rates. The slopes of the lines correspond to the rates at 33 and 160 $\text{M}^{-1}\text{s}^{-1}$ for scans at 100 and 2000 mV/s, respectively.

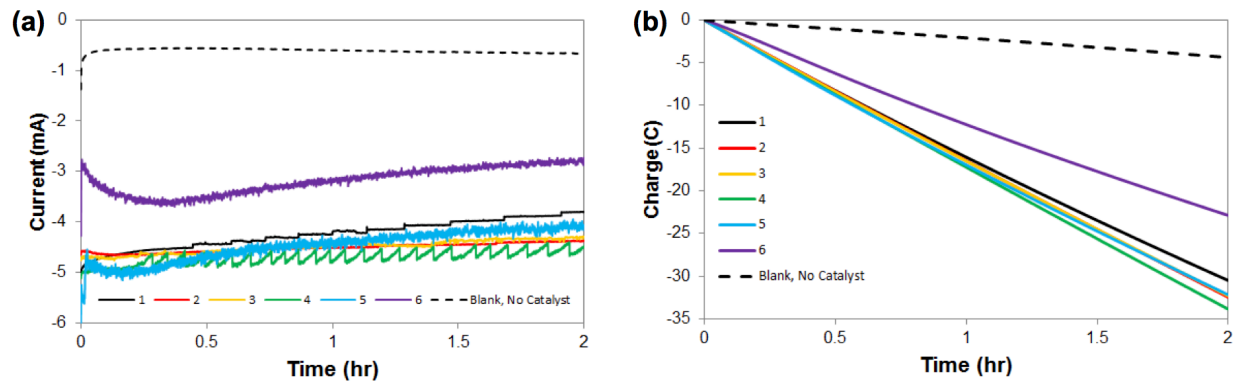


Figure S42. Overlay of current (a) and charge (b) traces for controlled potential electrolysis (CPE) experiments for complexes **1–6** measured at -2.8 V vs. $\text{Fc}^{+/0}$ over 2 hours. Electrochemical studies are performed in DMF solutions containing 0.1 M $[n\text{Bu}_4\text{N}][\text{PF}_6]$ under an atmosphere of CO_2 and in the presence of 2,2,2-trifluoroethanol (1.2 M) (dashed black), and catalyst (0.5 mM each).

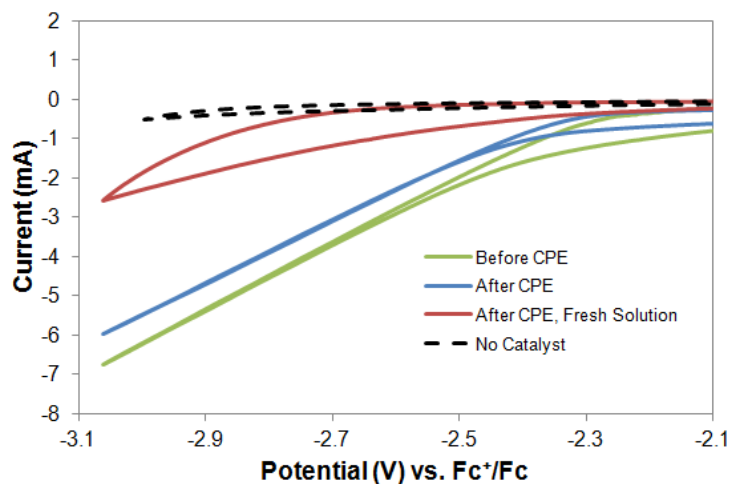


Figure S43. Cyclic voltammograms of **2** (0.5 mM) in a DMF solution containing $[n\text{Bu}_4\text{N}][\text{PF}_6]$ (0.1 M), 2,2,2-trifluoroethanol (1.2 M), and CO_2 (1 atm) before (blue) and after (green) controlled potential electrolysis (CPE). After the controlled potential electrolysis, the working electrode was rinsed (3×10 mL DMF) and its electrochemistry was measured in a fresh DMF solution containing $[n\text{Bu}_4\text{N}][\text{PF}_6]$ (0.1 M), 2,2,2-trifluoroethanol (1.2 M), and CO_2 (1 atm) – red. Scan rate is 100 mV/s.

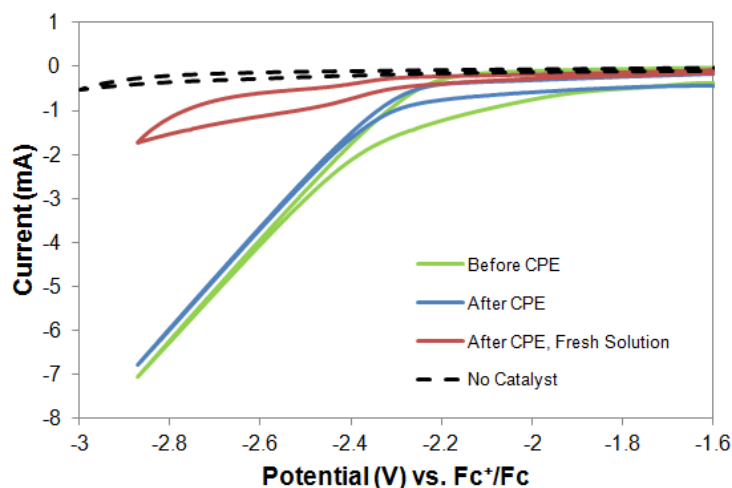


Figure S44. Cyclic voltammograms of **3** (0.5 mM) in a DMF solution containing $[n\text{Bu}_4\text{N}][\text{PF}_6]$ (0.1 M), 2,2,2-trifluoroethanol (1.2 M), and CO_2 (1 atm) before (blue) and after (green) controlled potential electrolysis (CPE). After the controlled potential electrolysis, the working electrode was rinsed (3×10 mL DMF) and its electrochemistry was measured in a fresh DMF solution containing $[n\text{Bu}_4\text{N}][\text{PF}_6]$ (0.1 M), 2,2,2-trifluoroethanol (1.2 M), and CO_2 (1 atm) – red. Scan rate is 100 mV/s.

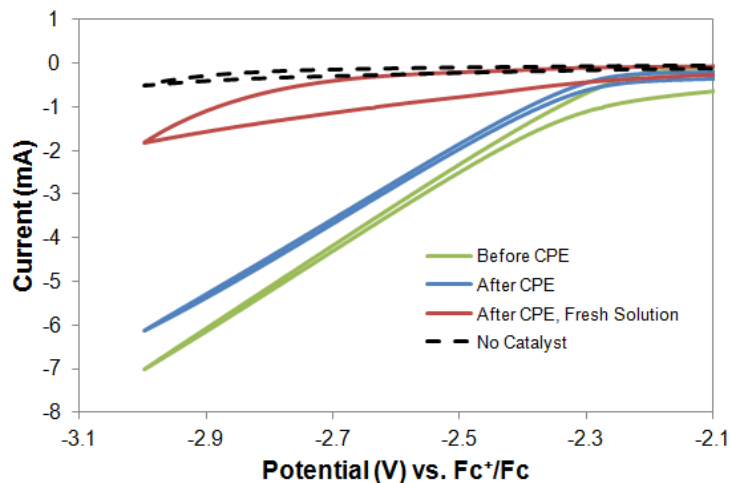


Figure S45. Cyclic voltammograms of **4** (0.5 mM) in a DMF solution containing [*n*Bu₄N][PF₆] (0.1 M), 2,2,2-trifluoroethanol (1.2 M), and CO₂ (1 atm) before (blue) and after (green) controlled potential electrolysis (CPE). After the controlled potential electrolysis, the working electrode was rinsed (3 × 10 mL DMF) and its electrochemistry was measured in a fresh DMF solution containing [*n*Bu₄N][PF₆] (0.1 M), 2,2,2-trifluoroethanol (1.2 M), and CO₂ (1 atm) – red. Scan rate is 100 mV/s.

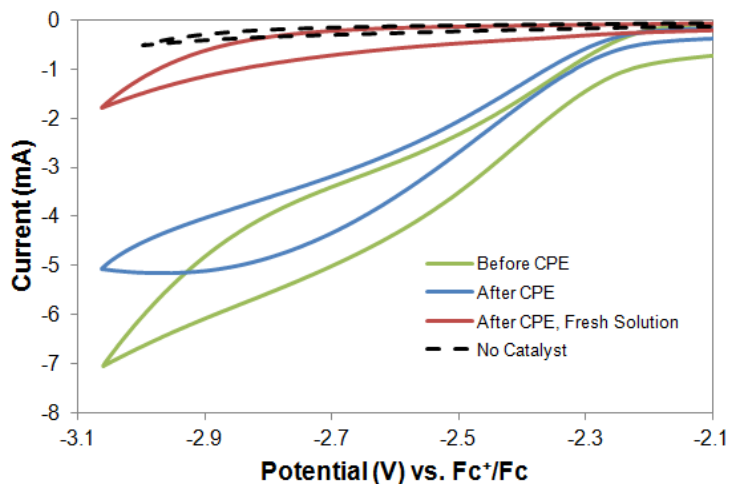


Figure S46. Cyclic voltammograms of **5** (0.5 mM) in a DMF solution containing [*n*Bu₄N][PF₆] (0.1 M), 2,2,2-trifluoroethanol (1.2 M), and CO₂ (1 atm) before (blue) and after (green) controlled potential electrolysis (CPE). After the controlled potential electrolysis, the working electrode was rinsed (3 × 10 mL DMF) and its electrochemistry was measured in a fresh DMF solution containing [*n*Bu₄N][PF₆] (0.1 M), 2,2,2-trifluoroethanol (1.2 M), and CO₂ (1 atm) – red. Scan rate is 100 mV/s.

Table S8. Summary of CPE results for complexes **1–6**. Overall TON is calculated as mol_{CO}/mol_{catalyst}. TOF_{CPE} (s⁻¹) is calculated as described previously, in eq. 6. TON_{CPE} is calculated by multiplying TOF_{CPE} (s⁻¹) with time for CPE studies (2*3600 s).

Complex	FE (%)	Charge (C)	Overall TON	TOF _{CPE} (s ⁻¹)	TON _{CPE}
1	98	30.9	10	170(20)	1.2(1)×10 ⁶
2	98	32.5	11	190(20)	1.3(1)×10 ⁶
3	98	32.3	10	190(20)	1.3(1)×10 ⁶
4	98	30.0	10	160(20)	1.1(1)×10 ⁶
5	90	32.2	7	155(20)	1.1(1)×10 ⁶
6	36	22.8	2	12.4(1)	9.0(9)×10 ³

Density functional calculation details

Density Functional Theory (DFT) calculations are performed using the Molpro 2015.1⁵ and Q-Chem 5.0⁶ software packages. Geometry optimizations and frequency calculations employ Molpro, while implicit solvation calculations use the Q-Chem package (except where explicitly otherwise mentioned). All Molpro calculations use density fitting of both the Coulomb and exchange operators with the corresponding JKFIT basis.⁷

The B3LYP functional⁸⁻¹¹ is used for all calculations. The more computationally costly ω B97M-V functional¹² is tested on the CO₂ binding energies of complexes **1-6** and gives the same trend. Q-Chem calculations are done using the relatively-fine Lebedev exchange correlation grid¹³ with 75 radial and 302 points. The Molpro grid threshold is set to 10⁻¹⁰.

The 6-31+g*¹⁴ basis set is used for all optimizations and frequency calculations. Diffuse functions are included to properly treat the strong anionic character of the bound CO₂ (discussed in the next section). The larger double zeta basis set def2-SVPD as well as the higher-zeta basis sets def2-TZVPD and def2-QZVPD¹⁵ are tested, but SCF calculations in these bases do not converge for every geometry. (All SCF algorithms available in the Q-Chem 5.0 and Molpro 2015.1 packages are tested.)

In a modest basis set such as 6-31+g*, Basis Set Superposition Error (BSSE)^{16, 17} is a concern. To correct for BSSE, binding energy calculations are performed using the def2-TZVPD basis at the 6-31+g* optimized geometry. Binding energy calculations are also attempted using the def2-QZVPD basis at the 6-31+g* optimized geometry, but all fail except for the single case of complex **1^(I)-CO₂**. For this complex, the difference in binding energy between the quadruple and triple zeta bases is 0.37 kcal/mol, suggesting that the def2-TZVPD is sufficiently large to eliminate BSSE. The BSSE associated with the 6-31+g* basis for complex **1^(I)-CO₂** is also evaluated using the counterpoise method,¹⁸ yielding a correction of 4.4 kcal/mol. This is in excellent agreement with the BSSE correction derived from the energy difference between the 6-31+g* basis and the def2-QZVPD basis of 4.2 kcal/mol. BSSE-corrected binding energies are reported in Table S9 and main text Figure 2b.

Dimethylformamide solvation energies are computed using the SMD implicit solvent model¹⁹ in the 6-31+g* basis set using the Q-Chem 5.0 software package. Solvent calculations

are done, as recommended, at the gas phase optimized geometries. The SM12 model²⁰ is also tested and yields similar results, but the CM5 charge component of the model does not converge for all geometries.

When possible, geometry optimizations are started from crystal structure initial guesses, and the resulting DFT minima do not deviate qualitatively from the crystal structure geometries. All geometric minima are fully optimized to the default thresholds of the Molpro 2015.1 software package. Harmonic vibrational calculations verify that all optimized geometries are indeed. These vibrational calculations also provide finite temperature (300K) harmonic thermodynamic corrections.

Transition state searches are performed in three steps. First, the freezing string method²¹ (15 nodes, 3 gradient descent steps, LST coordinates) is used to estimate a minimum energy path. Then, the transition state is located using a minimum mode following algorithm from the highest-energy FSM image.²² Finally, vibrational calculations are used to verify that transition states are first-order saddle points.

The geometries of complexes $1^{(II)}$ - $6^{(II)}$ and $1^{(I)}$ - $6^{(I)}$ are computed in the presence and absence of explicit solvent molecules in the axial positions. These are found to bind only weakly (binding energy of 1-2 kcal/mol and bond length of 2.5-3 angstroms) and to not affect the overall energetics of reduction. Therefore, they are not included in further calculations for the sake of computational efficiency.

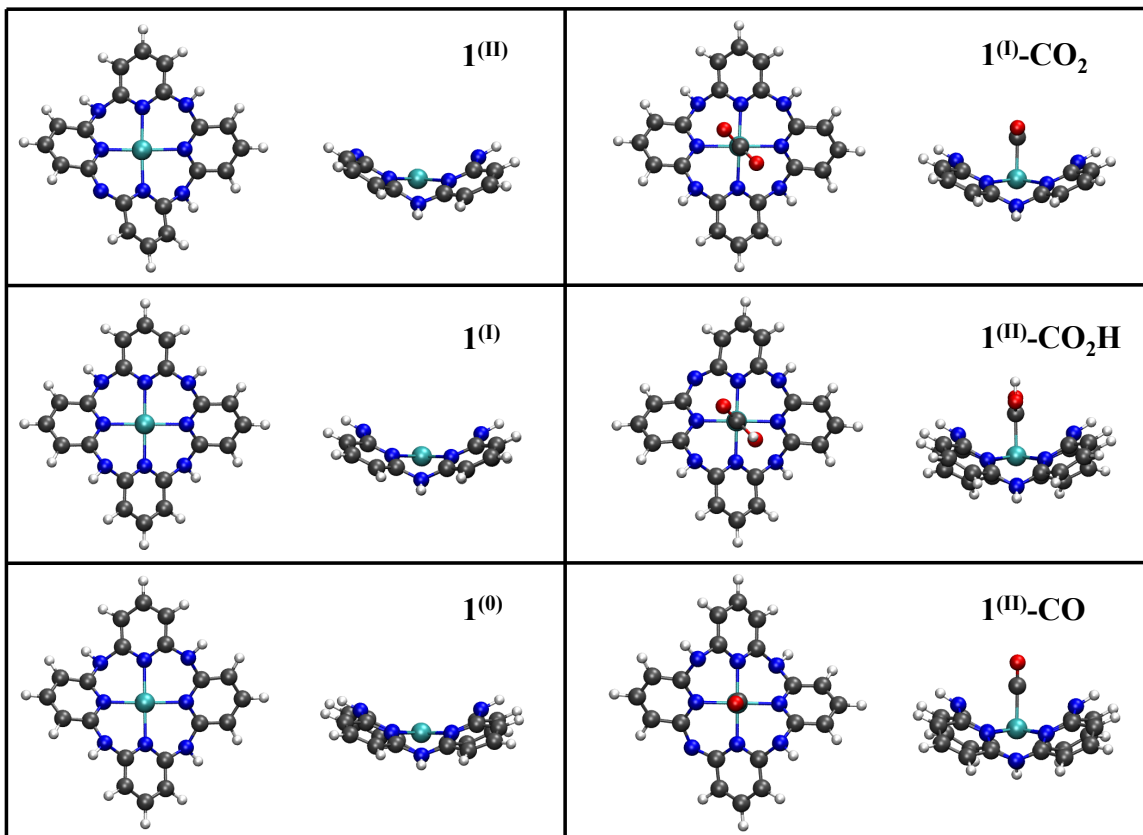


Figure S47. Top and side views of the optimized geometries of relevant minima for the reaction mechanism proposed in main text Figure 3 for complex **1**. The geometries for intermediates corresponding to complexes **2-6** are isostructural.

For complexes $1^{(II)}$ - $6^{(II)}$, the experimentally measured quartet spin state of complex $1^{(II)}$ is used. For complexes $1^{(I)}$ - $6^{(I)}$, the experimentally measured triplet spin state of complex $1^{(I)}$ is used. For all other complexes, cobalt has 9 d electrons, resulting in a doublet spin state. This assignment is also tested by computing the energies of the quartet complexes, which are in all cases found to be significantly higher.

Geometries of all structures mentioned in this study are included at the end of this document.

Computed reduction potential of $1^{(II)}$ - $6^{(II)}$.

The experimentally observed trend in reduction potentials of complexes $1^{(II)}$ - $6^{(II)}$ is explained by two effects: (i) the addition of electron-rich methyl groups is expected to shift potentials negatively and (ii) alkylation causes a decrease in solubility, shifting potentials positively. To disentangle these effects, DFT calculations – which contain electronic effects but not solubility effects – are performed.²³

The electronic energies and free energies of solvation for the $Co^{(II)}$ and $Co^{(I)}$ species are computed separately, and then subtracted to yield the implicit solvent estimate of the $Co^{(II)}$ reduction potential.^{24, 25} Increasing methylation shifts the reduction toward more negative potentials. To determine whether this effect is due to increased electron donation by the methyl substituents, the CHELPG²⁶ charge of the central cobalt atom is computed. In Figure S48, it can be seen that increasing methyl substitution increases with the charge on cobalt, which in turn shifts the reduction potential negative.

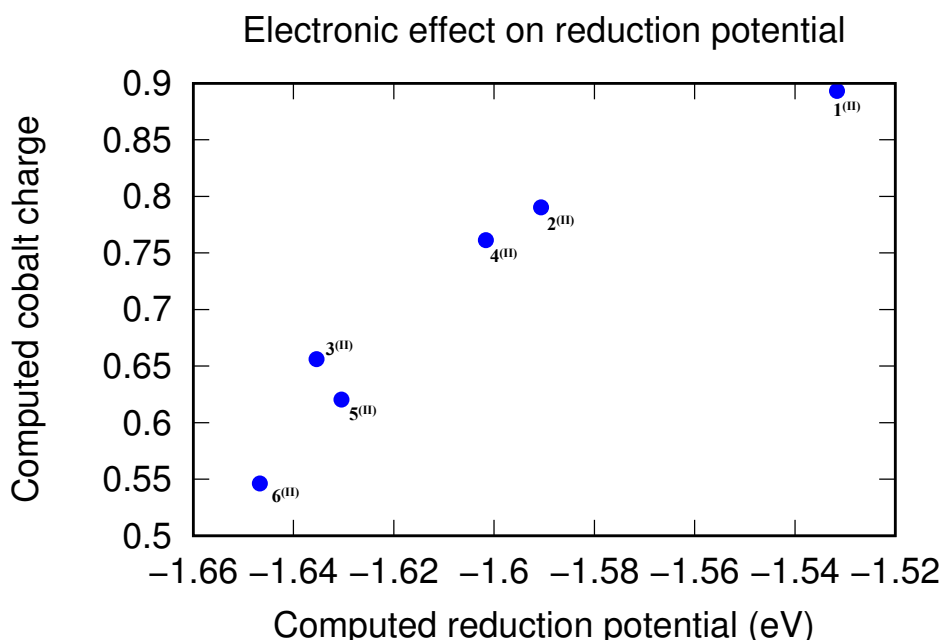


Figure S48. Comparison of computed reduction potential to computed charge on the central cobalt atom for complexes $1^{(II)}$ - $6^{(II)}$. Reduction potentials are referenced to the ferrocene/ferrocenium couple as computed using the same DFT model.

Density functional calculations on the binding of CO₂

Initial guess geometries for each $X^{(I)}$ -CO₂ adduct ($X=1-6$) are generated starting from the corresponding optimized $X^{(0)}$ geometry. The C atom of the ligand is placed at a distance of 2 angstroms from the Co atom of the complex. Binding energies and geometric parameters for complexes $1^{(I)}$ -CO₂ through $6^{(I)}$ -CO₂ are given in Table S9. Despite a range of 12 kcal/mol in binding energy, the adducts are largely isostructural, with similar C-Co bond lengths and O-C-O bond angles.

Upon binding, the CO₂ ligand bends and assumes the geometry of the gas phase CO₂ anion. In complex $1^{(I)}$ -CO₂, the C-O-C angle is 136 degrees (compared to 137 degrees in the gas phase anion). Similarly, the C-O bond length extends from the gas phase value of 1.17 Å to 1.24 Å to match that of the gas phase anion. This anionic character is further confirmed by CHELPG atomic charge analysis. Very similar results are found for complexes $2^{(I)}$ -CO₂ through $6^{(I)}$ -CO₂ and these results are summarized in Table S9.

Complex	Binding energy (kcal/mol)	C-Co bond length (Å)	O-C-O angle (degrees)	C-O bond length (Å)	CO ₂ charge
$1^{(I)}$ -CO ₂	-11.8	2.06	135.9	1.24	-0.70
$2^{(I)}$ -CO ₂	-9.9	2.07	135.8	1.24	-0.65
$3^{(I)}$ -CO ₂	-6.1	2.17	141.2	1.22	-0.49
$4^{(I)}$ -CO ₂	-5.3	2.15	140.3	1.22	-0.57
$5^{(I)}$ -CO ₂	+0.3	2.16	140.3	1.22	-0.52
$6^{(I)}$ -CO ₂	-0.4	2.14	139.3	1.23	-0.57
CO ₂ (g)			180.0	1.17	0
CO ₂ ⁻ (g)			136.1	1.24	-1

Table S9. CO₂ binding properties for complexes $1^{(I)}$ -CO₂ through $6^{(I)}$ -CO₂. Charges were computed using the CHELPG scheme. Gas phase geometries computed at the same level of theory are included for comparison.

The C-Co bond length changes by 0.1 Å between complexes $1/2^{(I)}$ -CO₂ and $3-6^{(I)}$ -CO₂, suggesting these groups of complexes may correspond to different potential energy minima. To test this possibility, the CO₂ bond lengths in complexes $3-6^{(I)}$ -CO₂ were changed to 2.06 Å. Following optimization from this set of initial guesses, all four complexes relax to their previous geometry. This suggests that all structures reported in Table S9 represent the same qualitative minimum.

The possibility of intramolecular hydrogen bonding is investigated in complex $1^{(I)}$ -CO₂. The CO₂ ligand is rotated 90 degrees and the pendant nitrogen centers were umbrella flipped to yield guess geometries for either one or two intramolecular hydrogen bonds. Both cases are found to be unfavorable. Formation of one intramolecular hydrogen bond incurs an energy penalty of 5.2 kcal/mol, while formation of two incurs a penalty of 6.5 kcal/mol. The transition states for these rearrangements are also found. These results are summarized in Figure S49.

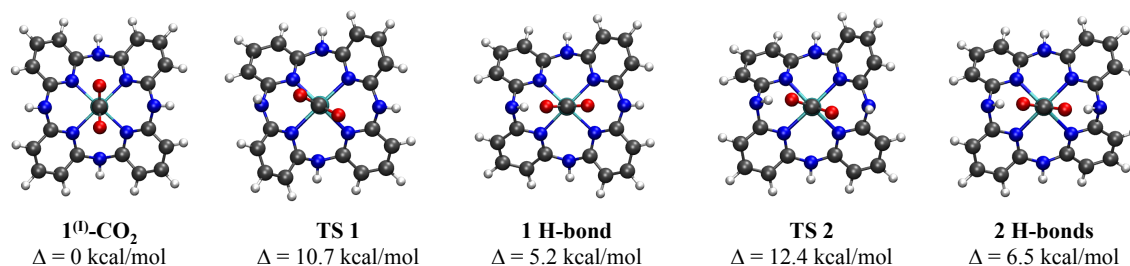


Figure S49. Geometries and energies for intramolecular hydrogen bonding between CO₂ and the amine protons in complex **1⁽⁰⁾-CO₂**.

Embedded multireference calculations on the favorability of hydrogen bonding in complex **1⁽⁰⁾-CO₂**

The previous section employs DFT to draw conclusions about rearrangement barriers and hydrogen bond strengths in complexes **X⁽⁰⁾-CO₂** (**X=1-5**). While DFT has been used to study small molecule reactions on cobalt complexes and surfaces,²⁷⁻³⁶ it can be inconsistent for reaction barriers in organometallic complexes.³⁷⁻⁴¹ Further, the geometry and strength of hydrogen bonds can be strongly functional dependent.^{42, 43} To verify that DFT is adequate to describe intramolecular hydrogen bonding and associated rearrangements in complexes **1⁽⁰⁾-CO₂**, accurate embedded wavefunction-in-DFT calculations on the formation of one hydrogen bond are performed. (Specifically, the first three structures in Figure S49 are considered.)

Projection-based embedding^{44, 45} calculations are performed in the MOLPRO 2017.0 software package. Calculations are performed in the def2-TZVP basis set. (All other parameters are the same as those used throughout the text.) B3LYP Kohn-Sham occupied orbitals are localized by the intrinsic bond orbitals procedure,⁴⁶ and the embedded localized orbitals are listed in Table S10. These orbitals correspond to the cobalt center, its four bonding nitrogens, the CO₂ ligand, and the hydrogen-bonding amines. The projector weight is set to 10⁶ Hartree, which results in B3LYP-in-B3LYP embedding errors on the order of 0.001 kcal/mol. To reduce the size of the virtual space, atomic orbital truncation⁴⁷ is performed with a charge threshold of 0.001 electrons, resulting in the retention of 713 of 1102 basis functions. MP2⁴⁸-in-B3LYP calculations confirm reaction energy convergence with respect to the atomic orbital truncation threshold.

Structure	Embedded localized molecular orbitals
1^(I)-CO₂	1, 2, 3, 4, 5, 6, 7, 8, 9, 12, 13, 14, 15, 24, 37, 38, 39, 40, 41, 42, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 59, 61, 62, 67, 68, 69, 70, 79, 80, 93, 94, 95, 96, 99, 100, 101, 102, 103, 104, 105, 114, 115, 116, 117, 118, 119, 120, 121
TS 1	1, 2, 3, 4, 5, 6, 7, 8, 11, 12, 13, 14, 15, 24, 37, 38, 39, 40, 41, 42, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 56, 61, 62, 67, 68, 72, 76, 79, 80, 93, 94, 95, 96, 99, 100, 101, 102, 103, 104, 105, 114, 115, 116, 117, 118, 119, 120, 121
1 H-bond	1, 2, 3, 4, 5, 6, 7, 8, 11, 12, 13, 14, 15, 24, 37, 38, 39, 40, 41, 44, 45, 46, 47, 48, 49, 50, 51, 52, 54, 58, 60, 61, 62, 63, 64, 73, 76, 77, 78, 93, 94, 95, 96, 97, 100, 101, 102, 103, 104, 105, 114, 115, 116, 117, 118, 119, 120, 121

Table S10. Localized molecular orbital numbers in the embedded subsystem for each geometry considered. The structure names refer to those of Figure S49.

Embedded coupled cluster singles and doubles^{49, 50} calculations are performed. As multireference character is always a concern in transition metal complexes, the T1 diagnostic⁵¹ is computed and found to be at least 0.07. This value exceeds both the standard threshold of 0.02 and the threshold of 0.05 suggested for first-row transition metals in Ref.⁵², indicating strong multireference character.

To treat this multireference character, embedded multireference configuration interaction singles and doubles (MRCISD)^{53, 54} are performed with a complete active space self-consistent field (CASSCF)^{55, 56} reference. The active space contains nine electrons in nine orbitals. Two factors suggest this active space is sufficiently large. First, the largest active space (at any geometry) determined by the unrestricted natural orbital complete active space method of Bofill and Pulay⁵⁷ is only three electrons in three orbitals. Second, the CAS(9,9) canonical orbital populations are at most 1.98 for the lowest-energy orbital and at least 0.03 for the highest-energy orbital across all geometries. Multireference character is confirmed by substantial deviations from integer occupations within the canonical orbitals.

Embedded calculations increase the energy penalty for the formation of one hydrogen bond by 1.0 kcal/mol to 6.2 kcal/mol and decrease the associated barrier for this process by 2.8 kcal/mol to 7.9 kcal/mol. Our qualitative conclusions remain unchanged: formation of intramolecular hydrogen bonds is thermodynamically unfavorable and CO₂ binds without hydrogen bonding.

Structure of the CO₂H adduct

After protonation, the CO₂H adduct retains the same bonding geometry as the CO₂ adduct. The C-Co bond length does not significantly change for complexes **1^(III)-CO₂H** and **2^(II)-CO₂H**. In the remaining four complexes, the C-Co bond contracts by ~0.1 Å, resulting in a tight distribution of C-Co bond lengths for all six complexes that ranges only over 0.02 Å. The geometric parameters of the CO₂H ligand are also nearly identical, resulting in isostructural adducts. This is reflected in the overall protonation energies of the CO₂H adducts, which vary little across the series (main text Figure 4), and in the experimental observation that the overall

rate depends only on the number of pendant amines (main text Figure 2a). Geometric parameters are presented in Table S11.

The CO₂H ligand resembles the gas phase anion (Table S11), though not as precisely as does the CO₂ ligand (Table S9). Focusing in particular on complex **1^(II)-CO₂H**, the two C-O bond lengths lie between the gas phase neutral and anion values. The bond angle of 116 degrees resembles that of the gas phase anion (112 degrees) more than that of the gas phase neutral molecule (130 degrees). The CHELPG-computed ligand charge reduces from -0.70 in complex **1^(II)-CO₂** to -0.32 in complex **1^(II)-CO₂H**. Overall, we conclude that the CO₂H ligand is less strongly anionic than the CO₂ ligand. This agrees with the computed overall energy of protonation being less favorable in the CO₂ adduct than in the CO₂H adduct (main text Figure 4).

Complex	C-Co bond length (Å)	O-C-O angle (degrees)	C=O bond length (Å)	C-OH bond length (Å)	CO ₂ H charge
1^(II)-CO₂H	2.06	116.3	1.22	1.41	-0.32
2^(II)-CO₂H	2.07	116.4	1.22	1.41	-0.27
3^(II)-CO₂H	2.08	116.8	1.23	1.40	-0.22
4^(II)-CO₂H	2.07	116.5	1.23	1.39	-0.30
5^(II)-CO₂H	2.08	116.5	1.23	1.40	-0.32
6^(II)-CO₂H	2.06	117.2	1.22	1.40	-0.27
CO₂H (g)		130.1	1.19	1.33	0
CO₂H⁻ (g)		112.2	1.24	1.45	-1

Table S11. Geometric and charge properties of complexes **1^(II)-CO₂H** through **6^(II)-CO₂H**. Charges are computed using the CHELPG scheme. Gas phase geometries computed at the same level of theory are included for comparison.

Effect of solubility on the first protonation energy

Main text Figure 4 presents the computed energy of protonation for complexes **1-6**. Notably, there is a large change in the first protonation energy (about 7 kcal/mol) between complexes **1** and **2** versus **3-6**.

It has previously been reported that the methylation of amines on methyl cyclam complexes can shift their reduction potential positively due to a decrease in the solvation energies associated with the ligand.²³ Experimentally, ligands **L¹⁻²** are only soluble in polar organic solvents (acetone, methanol, etc), while ligands **L³⁻⁶** are readily soluble in non polar solvents like dichloromethane, indicating that there is a dramatic shift in solvation energies going from **L²** to **L³** and onward. We suspect that the change in the calculated free energy of the first protonation event is due to that same difference in solvation energy that we incur upon methylation.

Computations on the first protonation reaction energy with and without solvation are shown below. In gas phase (without solvent), the reaction energy ranges over 2.3 kcal/mol and complexes **1** and **2** do not cluster when compared to complexes **3-6**. This agrees with the experimental solubility discussed above.

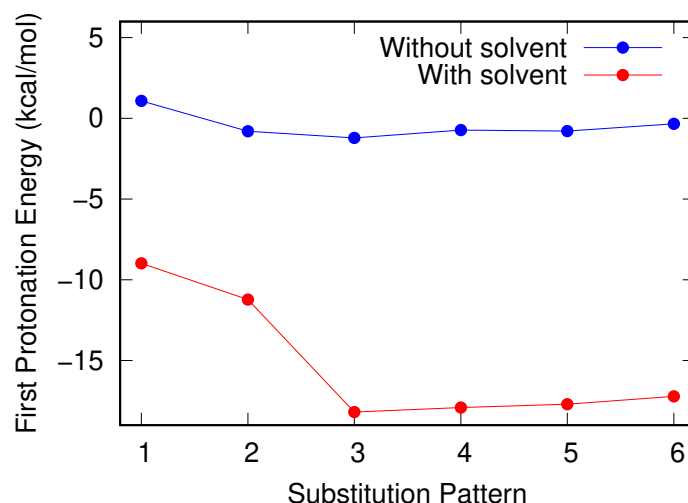


Figure S50. Calculated first protonation energy for complexes **1-6** with and without implicit solvent.

Mechanism of the second protonation: intra- versus intermolecular proton transfer.

As discussed in the main text, a candidate mechanism for the rate-limiting protonation of the CO₂H ligand is intramolecular proton transfer from a pendant amine. This pathway proceeds in two steps and is illustrated for complex **1^(III)-CO₂H** in Figure S51. First, the CO₂H ligand rotates roughly 45 degrees toward the pendant amine, which simultaneously undergoes an umbrella flip. This step is energetically unfavorable by 10.3 kcal/mol and has a barrier of 15.2 kcal/mol. The second step is proton transfer, which is strongly energetically favorable and incurs an additional barrier of 3.9 kcal/mol. After proton transfer, the C-OH₂ bond breaks spontaneously to generate water.

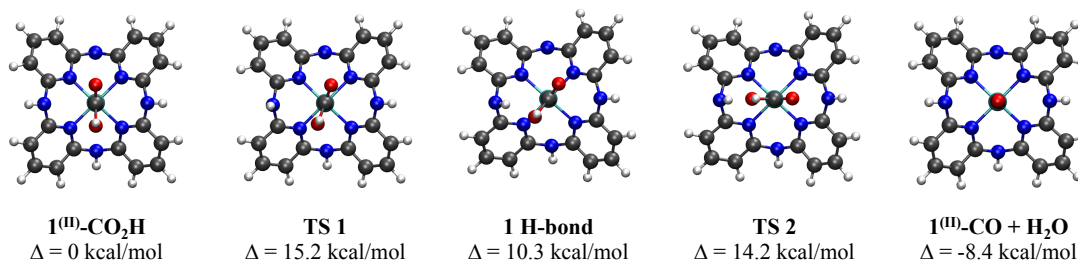


Figure S51. Geometries and energies for intramolecular proton transfer from a pendant amine to the COOH in complex **1^(III)-CO₂H**. This is a candidate mechanism for the rate-limiting protonation step.

This intramolecular mechanism is not the primary catalytic pathway for two reasons. First, a lower energy pathway involving acid stabilization is available. Second, this pathway does not have an explicit acid dependence, contradicting experiment. A possible modification to the intramolecular mechanism that could allay both concerns comes through acid stabilization of the transition state. To test this possibility, complex **1^(III)-CO₂H** and its intramolecular hydrogen-bonding intermediate (first and third structures in Figure S51) are reoptimized in the presence of

an explicit water molecule – representing the acid – placed near the pendant amine. The explicit acid molecule raises the energy of the intermediate from 10.3 kcal/mol to 11.4 kcal/mol, eliminating this explanation. The geometry of the acid-stabilized hydrogen-bonding intermediate is shown in Figure S52.

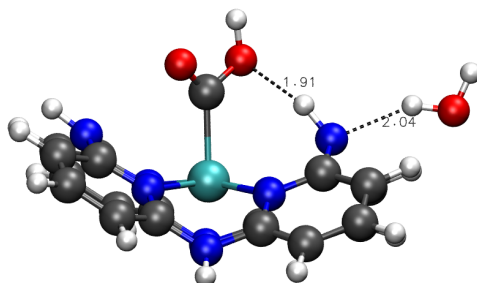


Figure S52. Structure of $1^{(III)}\text{-CO}_2\text{H}$ forming one hydrogen bond between the pendant proton and the CO_2H group in the presence of an explicit acid molecule. For computational efficiency, water stands in for TFE. Hydrogen bond are indicated by dotted lines labeled by their corresponding bond lengths in Ångstroms.

Comparison of the intra- versus intermolecular mechanism for the first protonation

Step	First protonation	Second protonation
<i>Intramolecular</i>		
H-bond formation barrier	10.7	15.2
H-bond formation energy	5.2	10.3
Proton transfer barrier	5.7	3.9
<i>Intermolecular</i>		
TFE binding energy	-15.6	-4.3

Table S12. Comparison of intermediates for intra- and intermolecular protonation between the first and second protonation steps for complexes $1^{(I)}\text{-CO}_2$ (first protonation) and $1^{(III)}\text{-CO}_2\text{H}$ (second protonation). Energies are listed in kcal/mol and referenced to $1^{(I)}\text{-CO}_2$ and $1^{(III)}\text{-CO}_2\text{H}$ in their corresponding energy minima with no intramolecular hydrogen bonds. These intermediates are depicted for complex $1^{(III)}\text{-CO}_2\text{H}$ in main text Figure 5.

Calculation of proton free energy

In main text Figure 4, the thermodynamic driving forces for both protonation steps are reported. While the arguments made therein rely only on the relative reaction energies between the first and second protonations and among complexes, it can be helpful to have an absolute

energy. The incomputable (at the DFT level) component of such an energy is the free energy of the proton in the conditions of the experiment. We thus turn to experimental measurements for a reference. However, (to our knowledge) there are no measurements of the free energy of the proton in DMF, but there are measurements in dimethyl sulfoxide, a polar aprotic solvent with a similar dielectric constant (DMSO=48, DMF=37). Four measurements of the proton free energy in DMSO are reported and we use the mean of their range, -271.0 kcal/mol.⁵⁸ We convert from DMSO to DMF by computing the difference in protonation energy in these two solvents at the DFT level. This correction term is small; for example, the correction for the first protonation of complex **1**^(I)-CO₂ is 0.5 kcal/mol. These small corrections are corroborated by CV experiments: substitution of DMF with DMSO in studies of complex **1** did not significantly change the position of the redox waves or their current densities.¹

The proton free energy is then adjusted to account for the presence of 1M 2,2,2-trifluoroethanol (TFE). Using the pKa of TFE in DMSO (-23.5)⁵⁹ and a temperature of 300K, the effect of the pH is found to be -14.8 kcal/mol.

Acidity of the intermediates

The acidity (pKa) of the intermediates was computed with reference to measured pKas for complexes **X**^(II), **X**=**1-5**. The pKa for general complex **Y** was computed as:

$$pK_a^{comp,Y} = pK_a^{expt,ref} + \frac{1}{kT \ln(10)} (G^{comp,Y} - G^{comp,ref})$$

where $kT \ln(10) = 1.364$ at room temperature and G represents the computed free energy. The computed pKas are shown in Table S13. Significantly, the pKa of complexes **X**^(II)-CO₂H (**X**=**1-5**) are consistent with single deprotonation under experimental conditions.

Complex	X ^(II)	X ^(I)	X ⁽⁰⁾	X ^(I) -CO ₂	X ^(II) -CO ₂ H
1	2.7	9.9	13.0	15.2	2.7
2	2.7	N/A	12.2	15.9	2.5
3	2.5	10.8	10.5	13.2	3.7
4	3.1	11.2	11.2	12.1	3.3
5	2.5	N/A	15.2	12.8	3.5

Table S13. pKa for intermediates of the catalytic cycle. Values for complexes **X**^(II) (italic) come from experimental measurements. The remaining values are computed with reference to these measurements. N/A indicates complexes where calculations failed to converge.

Analysis of the (E)ECEC mechanism for the second protonation step

The mechanism shown in Figure 3 of the main text depicts an EECC sequence, which involves two reduction steps followed by two chemical proton-transfer steps. As discussed in main text section “Nature of the rate-limiting protonation”, an alternative (E)ECEC mechanism (depicted in Figure S53) cannot be completely excluded, although DFT calculations suggest the EECC mechanism is more likely. The conclusions drawn in this work regarding the formation of a CO₂-bound pre-association complex and the nature of the rate limiting step are consistent with both the EECC and (E)ECEC pathways.

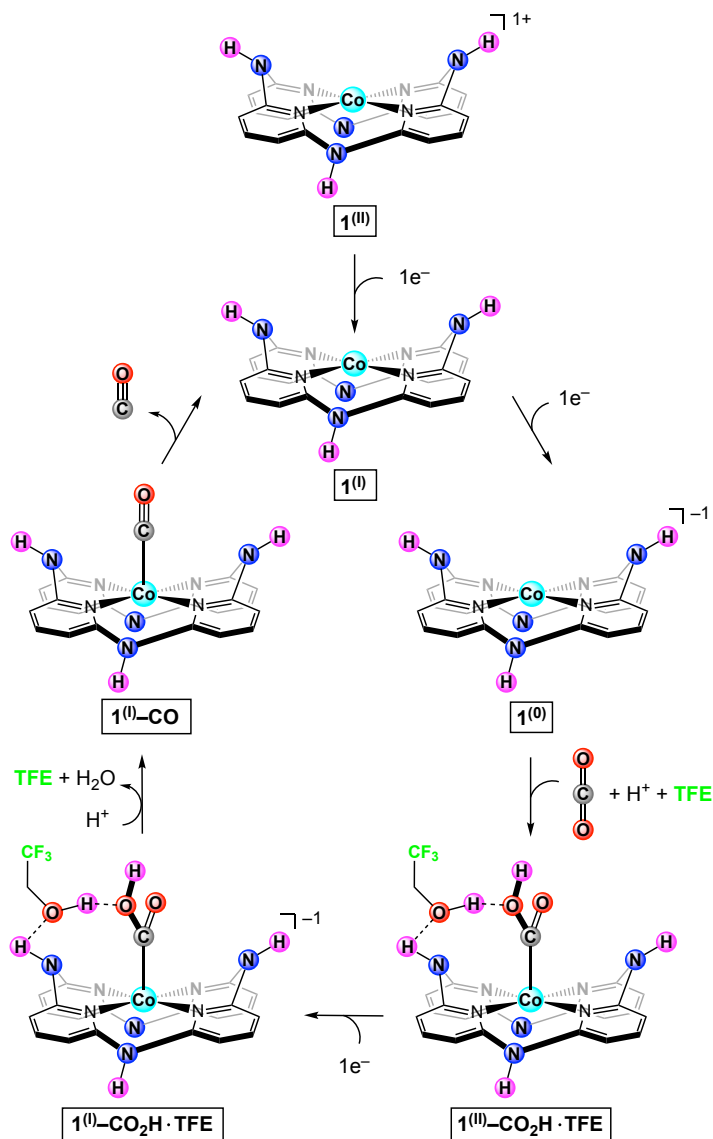
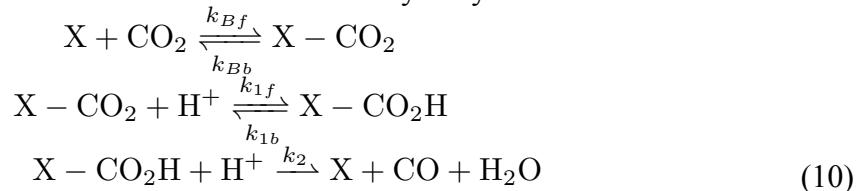


Figure S53. The alternative (E)ECEC catalytic cycle illustrated with complex **1**, where E = electrochemical, and C = chemical step.

Kinetics of the EECC mechanism

We introduce a mechanism for the kinetics of the catalytic cycle:



The first step represents potentially reversible CO_2 binding to complex $\mathbf{X}^{(0)}$ ($\mathbf{X}=\mathbf{1-6}$). The second step is the potentially reversible first protonation. The final step is the irreversible second protonation and regeneration of the catalyst. Based on computational results presented in the main text sections “Formation of the CO_2 -bound pre-association complex” and “Nature of the rate-limiting protonation step”, we assert that the second protonation is rate-limiting, and therefore k_2 is small compared to the other rate constants in this model.

This mechanism leads to the standard set of equations for the concentrations of the species involved in the reaction:

$$\begin{aligned}
 \frac{d[X]}{dt} &= -k_{Bf}[X][\text{CO}_2] + k_{Bb}[X - \text{CO}_2] + k_2[X - \text{CO}_2\text{H}][\text{TFE}] \\
 \frac{d[X - \text{CO}_2]}{dt} &= k_{Bf}[X][\text{CO}_2] - k_{Bb}[X - \text{CO}_2] - k_{1f}[X - \text{CO}_2][\text{TFE}] + k_{1b}[X - \text{CO}_2\text{H}] \\
 \frac{d[X - \text{CO}_2\text{H}]}{dt} &= k_{1f}[X - \text{CO}_2][\text{TFE}] - k_{1b}[X - \text{CO}_2\text{H}] - k_2[X - \text{CO}_2\text{H}][\text{TFE}] \\
 k_{cat} &= \frac{d[\text{CO}]}{dt} = k_2[X - \text{CO}_2\text{H}][\text{TFE}]
 \end{aligned} \tag{11}$$

In the experiments, the initial concentration of the catalyst is 0.0005 M, which is much smaller than the initial concentration of CO_2 (0.2 M) and TFE (1.2 M). We therefore consider the behavior of this mechanism over initial observation timescales where the concentration of reactants do not decrease appreciably:

$$\frac{d[\text{CO}_2]}{dt} = \frac{d[\text{TFE}]}{dt} \approx 0 \tag{12}$$

In the main text section “Nature of the rate-limiting protonation step,” we compute a strongly energetically downhill (~ 10 kcal/mol) first protonation reaction energy. We therefore argue that the first protonation is irreversible:

$$k_{1b} \approx 0 \tag{13}$$

Making the steady state approximation for the intermediates $\mathbf{X-CO}_2$ and $\mathbf{X-CO}_2\text{H}$, allows the rate equations to be solved analytically, yielding the rate law:

$$k_{cat} = \frac{k_2 k_{Bf} [\text{CO}_2] [\text{TFE}] [X]_i}{[\text{TFE}] k_{1f} + k_{Bb}} \tag{14}$$

In the limit that CO_2 binding is fast compared to the first protonation, this reduces to:

$$k_{cat} \approx k_2 K_B [\text{CO}_2] [\text{TFE}] [\text{X}]_i \quad (15)$$

where $K_B = k_{Bf}/k_{Bb}$ is the equilibrium constant associated with CO_2 binding. This final rate law agrees with the experimentally observed linear dependence of the rate on $[\text{CO}_2]$ and $[\text{TFE}]$ (figures S23 and S25). It is also a restatement of the rate law presented in the main text, which expands on the factors that contribute to k_2 and the CO_2 binding constant.

To verify that the approximations made in this derivation are reasonable, we also numerically solve the differential equations without invoking the steady state approximation. We begin with initial concentrations that reflect those in experiment: $[\text{X}]_i = 0.0005 \text{ M}$, $[\text{CO}_2]_i = 0.2 \text{ M}$, $[\text{TFE}]_i = 1.2 \text{ M}$, and all other initial concentration are zero. We then assign rates consistent with our mechanism of fast reversible CO_2 binding, an irreversible first protonation, and an irreversible, rate-limiting second protonation: $k_{Bf} = k_{Bb} = 100k_2$, $k_1 = 5k_2$, and $k_{1b} = 0$.

Time series for the concentrations of intermediates as well as the product CO are shown in Figure S54. The concentrations of catalytic intermediates rapidly reach a constant value, justifying the steady-state approximation made in the analytics above. After this point, production of CO is linear in time, as expected for a catalytic process in steady state.

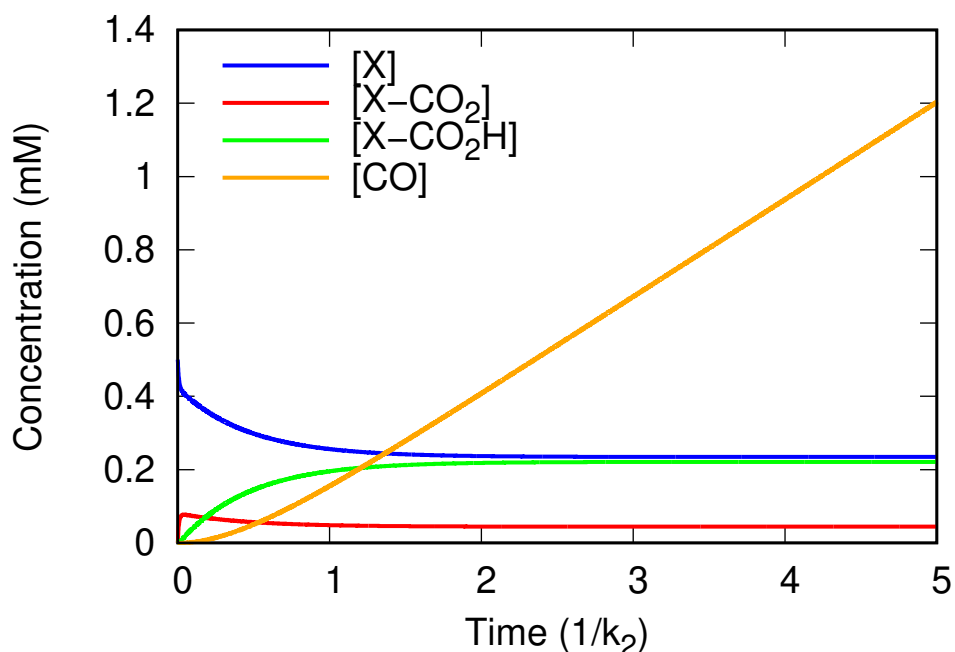


Figure S54. Time series for the concentrations of intermediates and CO from numerical simulation.

The dependence of the overall rate on the concentration of CO_2 and TFE is also tested numerically and presented in Figures S55 and S56. The same rates and initial concentrations as in the time series simulation are used (with the exception of the varying initial concentration of CO_2 or TFE). The rate is seen to be approximately linear in $[\text{CO}_2]$ and $[\text{TFE}]$. These trends become more linear as k_1/k_2 and k_{bB}/k_1 increase.

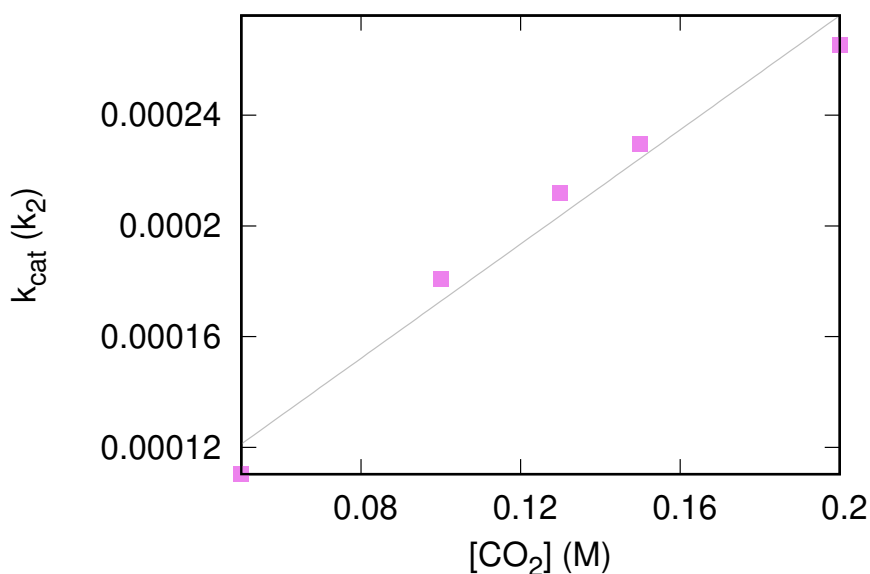


Figure S55. Overall rate as a function of CO₂ concentration computed numerically with the kinetic mechanism. Concentrations are chosen to match those in Table S5 and Figure S23. A linear fit is shown in gray.

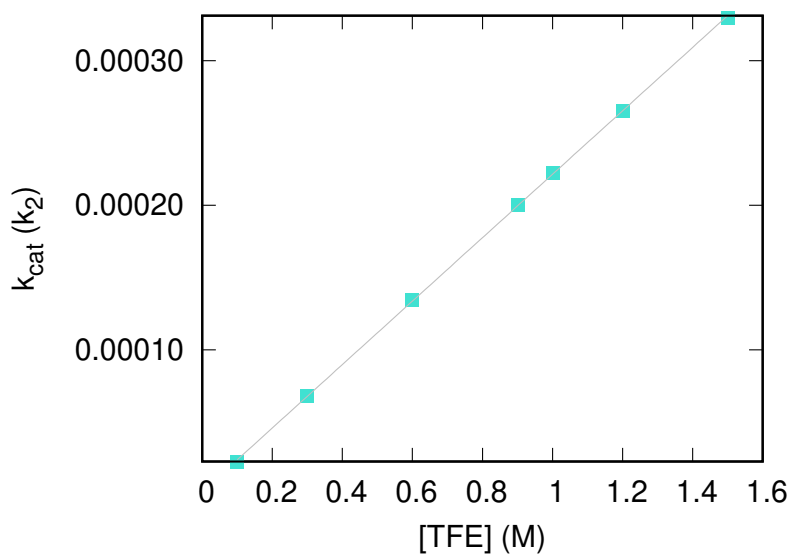


Figure S56. Overall rate as a function of TFE concentration computed numerically with the kinetic mechanism. Concentrations are chosen to match those in Table S6 and Figure S25. A linear fit is shown in gray.

These kinetic results (equation 15, and the assumptions that lead to it) are consistent with the experimental and computational results presented in this study. Specifically, the

experimentally observed linear dependence of the rate on $[\text{CO}_2]$ and $[\text{TFE}]$ in combination with the kinetic model suggests that: (i) CO_2 binding is fast and reversible; (ii) CO_2 binding is fast compared to the first protonation; and (iii) the first protonation is irreversible. Point (i) is further supported by the linear correlation of the computed CO_2 binding constant to the overall rate (Figure 2b). Point (iii) is further supported by the strongly downhill reaction energy for the first protonation (Figure 4). Taken together, these experimental, computational, and kinetic arguments form a consistent picture of the proposed CO_2 reduction mechanism (summarized in Figure 3).

Additional mechanisms captured by the rate model

This kinetic rate model (Equation 10 and 11) is flexible and can produce other rate dependence on $[\text{CO}_2]$ and $[\text{TFE}]$ that have been seen in other studies of CO_2 -to-CO reduction.⁶⁰ These cases occur if the first protonation is reversible instead of irreversible, or when CO_2 binding is irreversible instead of reversible.

For example, if CO_2 binding and the first protonation are reversible and very fast, then these two steps establish quasi-equilibrium:

$$\begin{aligned} K_B &= \frac{k_{Bf}}{k_{Bb}} = \frac{[\text{X} - \text{CO}_2]}{[\text{X}][\text{CO}_2]} \\ K_1 &= \frac{k_{1f}}{k_{1b}} = \frac{[\text{X} - \text{CO}_2\text{H}]}{[\text{X} - \text{CO}_2][\text{TFE}]} \end{aligned} \quad (16)$$

The rate law becomes:

$$k_{cat} = K_B K_1 k_2 [\text{X}]_i [\text{CO}_2] [\text{TFE}]^2 \quad (17)$$

which is first order in $[\text{CO}_2]$ and second order in $[\text{TFE}]$. This behavior has previously been seen in CO_2 -to-CO reduction in iron porphyrins.⁶⁰

If CO_2 binding and the first protonation are irreversible and very fast compared to k_2 , then all X is rapidly converted to $\text{X}-\text{CO}_2\text{H}$ which accumulates, waiting for the second protonation to occur. Each time the second protonation occurs, the resulting regenerated X is again rapidly converted to $\text{X}-\text{CO}_2\text{H}$. The result is a saturation of $[\text{X}-\text{CO}_2\text{H}]$:

$$\begin{aligned} [\text{X}] &= [\text{X} - \text{CO}_2] = 0 \\ [\text{X} - \text{CO}_2\text{H}] &= [\text{X}]_i \end{aligned} \quad (18)$$

and the corresponding rate law:

$$k_{cat} = k_2 [\text{X}]_i [\text{TFE}] \quad (19)$$

which is first order in $[\text{TFE}]$ and has no dependence on $[\text{CO}_2]$.

Representative geometries from density functional studies

Listed here are the optimized geometries and transition states computed with DFT and referred to throughout the text. “Deprotonated” refers to single deprotonation of the aminopyridine ligand at a pendant amine position.

```
H 2.5555691768 -0.1573065507 3.8218796098
C 1.8251205521 0.2640788207 3.1389635677
C 0.820186446 1.1084145469 3.5975283504
H 0.7411460957 1.3371108534 4.6560636391
C -0.0859102952 1.6582475862 2.6931960638
H -0.8929423299 2.3008426976 3.0293551339
C 0.0365359718 1.3225317482 1.3460918352
N 1.0223419096 0.5161514734 0.87886802
C 1.9102307245 0.0082126132 1.7676075333
C -1.6146395201 1.0372608925 -0.4837097387
C -3.0021136395 1.1564519284 -0.5410741943
H -3.5224094244 1.8505189288 0.1107004828
C -3.7021019433 0.3291499615 -1.4164880042
H -4.7849822928 0.3861539779 -1.4725816141
C -3.0081061586 -0.5715072885 -2.2168903164
H -3.5304507996 -1.2097171063 -2.9221411648
C -1.6134251021 -0.6035973963 -2.1341168538
N -0.9201047181 0.1781744161 -1.2711743819
N 1.2338286423 -0.4652658683 -3.1148114908
C 0.2353005115 -1.1577735563 -3.7148279069
C 0.3061832457 -1.5672837251 -5.0491626481
H -0.5137377281 -2.1182652624 -5.4982158804
C 1.4221431353 -1.2088821006 -5.7972095019
H 1.4955569301 -1.5004361429 -6.8405930739
C 2.4461280226 -0.47564537 -5.2017207645
H 3.3373775217 -0.2041990911 -5.7577618433
C 2.32343895 -0.1397692026 -3.8546198411
H 5.5758732824 -1.0319454941 1.243033488
C 5.1419953715 -0.7037965011 0.3041474301
C 3.7598977457 -0.5346477664 0.1854378946
N 3.1758456423 -0.1225971736 -0.9658628327
C 3.9745874624 0.1565612507 -2.0261680851
C 5.3635005251 0.0532263503 -1.9700205814
H 5.9680574918 0.2786184529 -2.8423183434
C 5.9468382819 -0.3933640271 -0.7864968093
H 7.0251128932 -0.5002577276 -0.7162787359
N -0.9021199235 -1.4752066504 -2.9652317899
H -1.512874638 -2.1209703736 -3.4532014773
N 3.3526110487 0.5718555171 -3.2154531835
H 4.0207835647 0.9481760989 -3.8798377716
N 2.9439260602 -0.8035271661 1.2894439536
N -0.8807869212 1.8332258607 0.4118702847
H -1.4460894377 2.5778334875 0.806146866
Co 1.1365452133 0.1367831159 -1.1452056658
H 3.4546024529 -1.2535290376 2.0410503415
```

Listing S1. Coordinates of **1^(II)**.

```

H 2.8141175162 0.0534622282 3.7527277849
C 1.999413346 0.3818608371 3.1153026371
C 1.0091967218 1.2659672851 3.5910627569
H 1.0466872498 1.6179978282 4.617909615
C 0.0050672516 1.6731333481 2.7491895962
H -0.7918628136 2.3323667249 3.0714873752
C -0.0717156697 1.1698883595 1.4148121044
N 0.9466477796 0.3563038566 0.9396559583
C 1.9333400179 -0.0180896408 1.7950679799
C -1.671887836 0.889502666 -0.3582356793
C -3.0506961528 1.1376626594 -0.6359890058
H -3.5599850746 1.8474504047 0.0046324521
C -3.6992274511 0.4405636869 -1.6238992364
H -4.7572450384 0.6004339592 -1.8103531368
C -2.9821099114 -0.4917542254 -2.4019150424
H -3.4639171583 -1.0477093361 -3.1998165451
C -1.6318920335 -0.6431183295 -2.1541831139
N -0.9629775472 0.0216693848 -1.1762555344
N 1.2025155172 -0.4985906237 -3.0769422057
C 0.2272605226 -1.2098029478 -3.6929390594
C 0.3213119311 -1.5973432722 -5.0381198983
H -0.4810744253 -2.1653955365 -5.4973113345
C 1.4231264095 -1.1865539984 -5.7739730085
H 1.5103990154 -1.4544977929 -6.8227371134
C 2.4168471314 -0.4240652652 -5.1615813919
H 3.2997350092 -0.1080852194 -5.7072764563
C 2.2749859038 -0.1197626671 -3.8078057666
H 5.581805246 -1.0969354805 1.2204330882
C 5.1346737461 -0.7491141376 0.2950077555
C 3.7436195023 -0.591968606 0.2024216426
N 3.1402023567 -0.1584559992 -0.9308329366
C 3.9209483061 0.1704760718 -1.9842834902
C 5.3129952581 0.0881616978 -1.9523368264
H 5.9003384107 0.3534852471 -2.8251289448
C 5.9188980696 -0.3924238292 -0.7923006669
H 6.9997270459 -0.4838605264 -0.7397655742
N -0.8918199546 -1.5610492821 -2.950492148
H -1.5103309917 -2.1744474449 -3.4684684551
N 3.2841762365 0.6112348458 -3.1572902076
H 3.9495333514 0.9949369638 -3.8188249316
N 2.9411263744 -0.8894483337 1.2955833251
N -1.1779858792 1.4869273205 0.7322088725
Co 1.0368671593 -0.0172669308 -1.0293460902
H 3.4737555512 -1.3015359504 2.0529708566

```

Listing S2. Coordinates of **1^(II)**, deprotonated.

```

H 2.3681989638 -0.3070427835 3.8224470482
C 1.6817407582 0.1613407158 3.1243637696
C 0.6541755255 0.9795104929 3.5691500348
H 0.507174339 1.1377775311 4.6334020502
C -0.1894001361 1.6064264694 2.6467968414
H -0.9980447658 2.2414598507 2.9853108995
C 0.0100283884 1.3635612942 1.2922365744
N 1.0125361045 0.5593182736 0.8466987708
C 1.8478500282 -0.0069969361 1.7433136152
C -1.6005800988 1.0723960486 -0.5023102941
C -2.9905755434 1.1015644699 -0.4753667267
H -3.5200740491 1.7882779906 0.1725054239
C -3.6935544379 0.1954856554 -1.2753731554
H -4.7793119179 0.1854031802 -1.2581133476
C -3.0038991446 -0.6855146607 -2.0947858939
H -3.5307494435 -1.3735807263 -2.7482191981
C -1.6037531701 -0.6330120457 -2.0991673806
N -0.91541234 0.2092699451 -1.2997261539
N 1.2305080258 -0.4348526546 -3.1253730505
C 0.2383431414 -1.145864906 -3.713181216
C 0.3142411604 -1.5719653688 -5.0431078961
H -0.5006081313 -2.1352766701 -5.4861635332
C 1.4291935315 -1.2173486073 -5.7936631912
H 1.5055319164 -1.522769872 -6.832861921
C 2.4509212454 -0.4729946963 -5.206279701
H 3.3430063489 -0.2077376565 -5.7639535525
C 2.3220446757 -0.1180370811 -3.8653829963
H 5.544872253 -1.006684593 1.2423832855
C 5.1167640153 -0.6746910658 0.3021604071
C 3.7350013497 -0.4996281385 0.1769327038
N 3.1622982836 -0.0789145546 -0.9765458162
C 3.9666152249 0.1906095547 -2.0346867204
C 5.3539002652 0.0778671571 -1.9732203756
H 5.964362 0.2960797777 -2.8432197194
C 5.9282131953 -0.3685459027 -0.7843261271
H 7.0055019449 -0.481147432 -0.7081129043
N -0.8955767135 -1.4710420698 -2.9629722104
H -1.4978244695 -2.1315497441 -3.4412665675
N 3.3452516505 0.6062405823 -3.2263942876
H 4.0145632426 0.980676284 -3.8908267477
N 2.9158516512 -0.7756794076 1.2759788641
N -0.8113821345 1.9459340562 0.291233474
Co 1.1325278691 0.2307122514 -1.1755258671
H 3.4197506576 -1.2344403056 2.0266123788
C -1.4068128654 3.2581578533 0.6130428026
H -1.7930723377 3.6958186255 -0.3093027141
H -0.6195049196 3.906738426 1.0015715443
H -2.2186711375 3.2046713929 1.3486987772

```

Listing S3. Coordinates of $2^{(II)}$.


```

H 2.3396826083 -0.3343456794 3.844034684
C 1.6672438182 0.1358864362 3.1337223427
C 0.6611872144 0.9892737515 3.551542733
H 0.5102790032 1.1768423496 4.610641613
C -0.1562282629 1.6197852161 2.6077159105
H -0.951199987 2.2828186966 2.9233905855
C 0.0481920243 1.3376772451 1.2598110585
N 1.0262207539 0.4980271433 0.8380070877
C 1.8448093806 -0.0653292199 1.753566032
C -1.5601066921 1.0432791148 -0.5318433319
C -2.9505130084 1.1085802354 -0.5052197064
H -3.462009927 1.8234031772 0.1260885857
C -3.6752223862 0.1967046802 -1.2796578384
H -4.7610623324 0.2137190003 -1.2625212715
C -3.0072008766 -0.718580667 -2.0740028044
H -3.5459609947 -1.410289162 -2.7136685798
C -1.6014376619 -0.696169955 -2.0846926347
N -0.893780143 0.146416136 -1.3005969371
N 1.2727614647 -0.6158305281 -3.0983402868
C 0.2059671792 -1.1780200012 -3.7235988561
C 0.156027681 -1.4243301996 -5.0820372674
H -0.7237303145 -1.8734749826 -5.531713496
C 1.2590225956 -1.0313371954 -5.8679931749
H 1.2399907821 -1.1894084457 -6.9424544354
C 2.3498479642 -0.4548421634 -5.2666257796
H 3.2315327639 -0.1599499834 -5.8227589718
C 2.3938796997 -0.2937823825 -3.8484903558
H 5.5183012438 -0.7210258915 1.4177857666
C 5.1105193405 -0.5089155444 0.4346147879
C 3.7461599149 -0.5253152905 0.2181766061
N 3.1707898151 -0.2658555503 -0.9846073557
C 3.9880723438 0.0013979721 -2.0728478595
C 5.397563256 0.1109374216 -1.871921706
H 6.0003511579 0.3559287772 -2.7380894135
C 5.948908426 -0.1624707305 -0.6451275877
H 7.0244611778 -0.1168942121 -0.5004804565
N -0.906833958 -1.5551229359 -2.9223464279
H -1.5244106894 -2.1846081878 -3.4212952982
N 3.5626586307 0.1128362533 -3.337390361
N 2.8890951072 -0.8580394758 1.3031122515
N -0.7645156045 1.9175513152 0.2521881505
Co 1.1955958545 0.0069541208 -1.1938826751
H 3.4059896578 -1.2790258774 2.0661381097
C -1.3366437796 3.2387005822 0.5488966764
H -1.7141141204 3.6675313584 -0.3816131969
H -0.5399720399 3.8815592615 0.9287454616
H -2.1525580808 3.2164740169 1.2838696232

```

Listing S4. Coordinates of $2^{(II)}$, deprotonated.

```

H 2.334269234 -0.3245558731 3.7806519233
C 1.6525575931 0.1549992137 3.0854556119
C 0.6255939152 0.9700485269 3.5367249598
H 0.4764227091 1.1159717892 4.6024320054
C -0.2172193289 1.607327436 2.6200989268
H -1.0278582501 2.2366699345 2.9645432864
C -0.0123564552 1.3812231302 1.2638205142
N 0.9934795598 0.5857287132 0.8120379308
C 1.8223648343 0.0009579123 1.7024037495
C -1.6161584961 1.100192111 -0.5390042717
C -3.0061372689 1.1229648921 -0.5192798086
H -3.5434312989 1.8043807574 0.1278142699
C -3.6991458704 0.2158257367 -1.3273858949
H -4.7849461326 0.2012116121 -1.3181169055
C -3.0005801107 -0.6626963948 -2.1417334906
H -3.5209516595 -1.3543232224 -2.7966265649
C -1.5999289061 -0.6057097554 -2.136594175
N -0.9228549551 0.245097327 -1.3369791879
N 1.2202615198 -0.3824230564 -3.1472261509
C 0.2712866385 -1.1583484695 -3.7120467129
C 0.4102247996 -1.674436573 -5.0081052841
H -0.3683220085 -2.2951941483 -5.4399902178
C 1.5398627099 -1.3326190205 -5.7359471429
H 1.669422594 -1.7091689483 -6.7462498046
C 2.5117435733 -0.5000578573 -5.1712332824
H 3.401045741 -0.2363414018 -5.7292638488
C 2.3256879185 -0.0543971852 -3.8677036302
H 5.4887386419 -1.2171602276 1.1229400127
C 5.0648303565 -0.8166734999 0.2075924399
C 3.6943093711 -0.5348656636 0.1222553771
N 3.1370544587 -0.033948812 -1.0003670222
C 3.9305199754 0.243337489 -2.0690771236
C 5.3029739518 0.0229957946 -2.0418816079
H 5.9200644999 0.2411260585 -2.9040671445
C 5.8667309072 -0.5269024491 -0.8860205175
H 6.9336262688 -0.7252042621 -0.8448152684
N -0.8861055736 -1.451047384 -2.9883486145
H -1.4815600362 -2.1221844134 -3.460041698
N 3.2695147632 0.7782589422 -3.2074439191
N 2.8843700626 -0.7747455112 1.2340269702
N -0.8309875619 1.9716106429 0.2630925245
Co 1.1257509298 0.3203566679 -1.2198396428
H 3.3780337407 -1.2508248246 1.9804760224
C -1.4339873654 3.277201138 0.5966143704
H -1.8192243916 3.7230488673 -0.3222649247
H -0.6516086568 3.9254781382 0.9954902147
H -2.2484168921 3.2116089936 1.3285207373
C 4.0655431848 1.676334629 -4.0671172497
H 3.3853043783 2.195306869 -4.7448996778
H 4.8289810921 1.1567934576 -4.6591849389
H 4.5543412956 2.4171221735 -3.4316161238

```

Listing S5. Coordinates of $3^{(II)}$.

```

H 2.3340036615 -0.3721642795 3.7147231307
C 1.6529428461 0.1359099854 3.0394403247
C 0.6684449019 0.9893030611 3.5171983831
H 0.5499034012 1.1380573181 4.5865125279
C -0.1712520734 1.6528208828 2.6227471436
H -0.9587631953 2.3018238228 2.983377578
C -0.0117456298 1.4174113431 1.2558995061
N 0.9641329844 0.5998860523 0.7796979152
C 1.781543806 -0.0172456344 1.6518284274
C -1.6311979954 1.108621761 -0.5177984008
C -3.0014887995 1.0440173695 -0.3868434257
H -3.5264921939 1.6525596509 0.3387520637
C -3.7040403597 0.1334193293 -1.2105604352
H -4.7831009559 0.0480484551 -1.1180291938
C -3.0221409961 -0.6313238384 -2.1213776801
H -3.5217101677 -1.322302222 -2.7900770709
C -1.6060488014 -0.4950046036 -2.2667570196
N -0.931022804 0.3520118828 -1.4068949612
N 1.190998051 -0.2697647893 -3.1984914185
C 0.1848014504 -1.0232162265 -3.7751753471
C 0.4386461852 -1.6557731369 -5.0324840964
H -0.3568899567 -2.2627449299 -5.4482713334
C 1.6206528926 -1.4400497668 -5.6925252341
H 1.8032888508 -1.9005342887 -6.6594017679
C 2.6095254121 -0.6082755442 -5.1164143107
H 3.5482548966 -0.429897782 -5.6258749355
C 2.3509034453 -0.0593732902 -3.8793038079
H 5.412959115 -1.2379224791 1.1242039229
C 5.0169586927 -0.8176086761 0.2052648358
C 3.6468832288 -0.5494838209 0.0784928495
N 3.1159753973 -0.021430262 -1.0390353087
C 3.9362844719 0.2792198841 -2.0804085068
C 5.3167420141 0.081966966 -2.0091911561
H 5.9532775279 0.3214542841 -2.8511221855
C 5.8514312135 -0.4851448827 -0.8526836016
H 6.9193528364 -0.6698472346 -0.7815525961
N -1.0451028295 -1.1782789723 -3.2714121551
N 3.304607833 0.7988054673 -3.2258589865
N 2.8050744129 -0.83445822 1.1595333125
N -0.843000107 2.007459796 0.2845504641
Co 1.0631686362 0.3900278001 -1.3190587665
H 3.2882899425 -1.3288208375 1.8997559714
C -1.4809018706 3.2802531161 0.6444339888
H -1.902592941 3.7178010705 -0.2624194858
H -0.717552134 3.9562886487 1.0374068532
H -2.2827958062 3.1827434224 1.3891853008
C 4.1182747926 1.6482966764 -4.104839309
H 3.4505797685 2.1426160822 -4.8129105371
H 4.883037136 1.1002873292 -4.6723587572
H 4.6115298126 2.4110942603 -3.4973327086

```

Listing S6. Coordinates of $3^{(II)}$, deprotonated.

```

H 2.388464671 -0.3037579253 3.8250373882
C 1.7123782181 0.1547574874 3.1156319013
C 0.7444610311 1.0543074261 3.5490059168
H 0.6484865478 1.2763635032 4.607808188
C -0.1006822299 1.673695841 2.6294406548
H -0.8691032432 2.3594133784 2.9622445522
C 0.0443307226 1.3551987923 1.2805963301
N 0.9934936076 0.4865555609 0.8505468283
C 1.8264779127 -0.1012612491 1.7442155232
C -1.5930720439 1.0565369984 -0.5031444378
C -2.9829276814 1.1085422387 -0.4750863866
H -3.5008012303 1.8002732881 0.1768952351
C -3.7015808081 0.2205402235 -1.2815056249
H -4.7873322702 0.2294041202 -1.2628498982
C -3.0292275367 -0.6647979326 -2.1114513445
H -3.569364836 -1.3356259998 -2.7719305937
C -1.6287346664 -0.6386056753 -2.1140410908
N -0.9274307398 0.1822785859 -1.3041108941
N 1.2144656526 -0.4780463997 -3.1200886896
C 0.214594653 -1.163983078 -3.7249322992
C 0.2946094339 -1.5738963823 -5.0589543473
H -0.5247945444 -2.1183066636 -5.5169341853
C 1.4229508602 -1.2274312053 -5.7946009102
H 1.5042980302 -1.5218558848 -6.8365872755
C 2.4492753541 -0.50351766 -5.1912601628
H 3.3480639111 -0.2422722459 -5.7400314675
C 2.3149118674 -0.161158436 -3.8464486803
H 5.4990925693 -0.9139896099 1.3275390614
C 5.0676004985 -0.6070199107 0.3837411162
C 3.6833515224 -0.5678740857 0.2115477181
N 3.1286976969 -0.1573197667 -0.9609586103
C 3.9386520615 0.1909154766 -1.9860331886
C 5.3310588442 0.2005925353 -1.8726666195
H 5.9528931823 0.4819108461 -2.7163634516
C 5.8911849301 -0.2018033001 -0.6669768695
H 6.9700739727 -0.2094762485 -0.5435632239
N -0.9300941764 -1.4793041764 -2.9844750602
H -1.5407756922 -2.1237263089 -3.4739138215
N 3.3385306401 0.5542020661 -3.2021201438
H 4.010397412 0.9339535938 -3.8604412498
N 2.8133050699 -0.9759182425 1.247548177
N -0.790298997 1.9237656203 0.2837146249
Co 1.1088486296 0.1315901877 -1.1597913186
C -1.3643892247 3.2507261727 0.5831504866
H -1.7583153972 3.6722051424 -0.3433318479
H -0.5642473543 3.8989743133 0.9451965946
H -2.1663178377 3.2234045051 1.3309804252
C 3.333066618 -1.9947982191 2.1808443557
H 3.84432252 -2.7650158998 1.6012708785
H 2.4880532762 -2.4580983123 2.6933182551
H 4.0263985931 -1.5894470853 2.9279094823

```

Listing S7. Coordinates of $4^{(II)}$.

```

H 2.5062805318 -0.1188611982 3.7497231455
C 1.8047312954 0.3299998829 3.0587419205
C 0.9116731785 1.3083868145 3.4896062119
H 0.9004520448 1.6096684595 4.5332019372
C 0.0279739668 1.8907880356 2.5898782525
H -0.6977748504 2.6206225894 2.9237346693
C 0.0541193335 1.4641990729 1.2545509878
N 0.9553237976 0.5454998708 0.8218985456
C 1.8062843521 -0.0198689485 1.7056148461
C -1.607956415 0.9986779317 -0.4588982391
C -2.9655911805 0.8649393077 -0.2680097221
H -3.4862566965 1.4492629995 0.4807137849
C -3.6599809538 -0.0771662087 -1.0645374153
H -4.7270944497 -0.2200413319 -0.9194669929
C -2.9876661135 -0.7895390159 -2.0230554797
H -3.4855808674 -1.4896253436 -2.6835956692
C -1.5890794619 -0.574577933 -2.2356934358
N -0.9108842673 0.272239019 -1.3766451175
N 1.2181613924 -0.3327449554 -3.1798240472
C 0.166354037 -0.9633048048 -3.8276345209
C 0.3512164238 -1.4123853544 -5.1697135654
H -0.4830825296 -1.921491621 -5.6369387832
C 1.5212270916 -1.1515746732 -5.8396501715
H 1.649267652 -1.4700187625 -6.8702644794
C 2.5668656351 -0.4729031031 -5.1812882386
H 3.510993363 -0.2741594117 -5.6782104412
C 2.3693545949 -0.104894938 -3.8646505045
H 5.3939734995 -1.1286623621 1.3356499702
C 5.0021217132 -0.769092624 0.3933770655
C 3.6268242744 -0.6297329307 0.1972974043
N 3.1151134607 -0.1581232812 -0.9673518622
C 3.9614458517 0.1598832911 -1.9725821708
C 5.3547488172 0.081770726 -1.8310129866
H 6.0040520491 0.3433643241 -2.6602127238
C 5.868201209 -0.3893899376 -0.6331930455
H 6.9422308465 -0.4729819304 -0.4949397652
N -1.0479521594 -1.1710587536 -3.3012009466
N 3.4110206727 0.5821600083 -3.1801526095
H 4.1216511069 0.9048970277 -3.8267283036
N 2.714570516 -0.9875001284 1.2140416412
N -0.8458619616 1.9528682661 0.3008937203
Co 1.0706416121 0.2107980892 -1.2529298614
C -1.5127557072 3.2288672924 0.5878927482
H -1.9955990604 3.573551389 -0.3279432529
H -0.7594934045 3.9641231404 0.8821162598
H -2.2717346542 3.1627746891 1.3795531326
C 3.148412023 -2.0260951175 2.1591798643
H 3.5845538387 -2.8501466548 1.5910151359
H 2.2694111933 -2.4002586021 2.6875968064
H 3.8831733586 -1.6776423004 2.8975763016

```

Listing S8. Coordinates of $4^{(II)}$, deprotonated.

```

H 2.42377852 -0.2410911106 3.7841444276
C 1.7377217539 0.2116994907 3.0805174334
C 0.774906564 1.1135211202 3.5206687007
H 0.6948606042 1.3441781198 4.5789535213
C -0.0883362529 1.7212591245 2.6098027461
H -0.8565654216 2.4037607929 2.949634584
C 0.0419257631 1.3956683638 1.2612259727
N 0.991634839 0.5316056123 0.8246530814
C 1.8317281241 -0.0576433847 1.709675815
C -1.6007522295 1.0686664722 -0.5151164576
C -2.990693848 1.092695902 -0.4781699785
H -3.519497332 1.7726943002 0.1774791718
C -3.6947020816 0.1910285895 -1.2833108609
H -4.780332522 0.1785782844 -1.2604523949
C -3.0091939238 -0.6829252545 -2.114129279
H -3.5399265646 -1.3667053854 -2.768985542
C -1.6084816468 -0.6311264674 -2.1229367361
N -0.9224138106 0.2103473108 -1.3215544582
N 1.2138761211 -0.4199825409 -3.1259976236
C 0.2634047884 -1.1850179117 -3.7023769531
C 0.4120678773 -1.6962677221 -4.9990623956
H -0.3659674182 -2.3090118444 -5.4431579862
C 1.5536587181 -1.3601819673 -5.7116200123
H 1.692639666 -1.7351674209 -6.7212594917
C 2.5244404164 -0.5341792751 -5.135093962
H 3.4201145287 -0.272961593 -5.6841655833
C 2.3267166553 -0.0890214105 -3.8326801755
H 5.488501279 -1.1403648945 1.1953557487
C 5.0513256583 -0.7618019512 0.280817164
C 3.6660507447 -0.5970506352 0.1596572474
N 3.120819922 -0.0948529926 -0.9746786814
C 3.9179284242 0.2557771769 -2.0142860523
C 5.3044882349 0.1358270138 -1.9475260823
H 5.9314356081 0.4079574092 -2.7867643774
C 5.8654427165 -0.3825861995 -0.7810006781
H 6.943038175 -0.4919152389 -0.7009196768
N -0.902780371 -1.4700652912 -2.9885246297
H -1.5025881791 -2.132567545 -3.4667764078
N 3.2600538354 0.753766505 -3.1696654188
N 2.8017044882 -0.9540649849 1.2153027541
N -0.8069238765 1.9506892447 0.2675559881
Co 1.1167098554 0.2383074584 -1.1933285822
C -1.403021814 3.2670177782 0.5699548084
H -1.8130720181 3.6795288452 -0.3535444267
H -0.6124849028 3.9310837998 0.9244875825
H -2.198019644 3.2253872618 1.3245712807
C 4.0378189832 1.6672121827 -4.0298745748
H 3.3501556867 2.1582875146 -4.7205976187
H 4.8228214242 1.1639948949 -4.6076248967
H 4.4967745136 2.4297729193 -3.3978368593
C 3.2871487582 -1.9883315051 2.1503210112
H 3.7477525999 -2.7903956336 1.5713439268
H 2.4301656913 -2.4033604617 2.6832768584
H 4.0136223183 -1.6094628659 2.8794490286

```

Listing S9. Coordinates of $5^{(II)}$.

```

H 2.4468444813 -0.2581354795 3.7223234247
C 1.7578214998 0.2192983312 3.0379910736
C 0.8385702105 1.156997672 3.4998080054
H 0.794020404 1.394198581 4.5589349456
C -0.0279251944 1.7837344214 2.6107218837
H -0.7718382016 2.4850590461 2.9655748504
C 0.0470006561 1.4419206666 1.2554924832
N 0.9679313641 0.5580005424 0.7972989757
C 1.8027462609 -0.05231216 1.6655245826
C -1.6123168399 1.0724371449 -0.487152063
C -2.9810797633 1.0025936519 -0.3399384503
H -3.5002320886 1.6106908304 0.3904409933
C -3.6893994948 0.0906316075 -1.1575186433
H -4.7670879522 0.001994431 -1.0526274059
C -3.0171799977 -0.6703505533 -2.0795011165
H -3.524403546 -1.3594521512 -2.744438551
C -1.6029778268 -0.5325896667 -2.2384743055
N -0.9233949895 0.3129900312 -1.3814368897
N 1.1925385136 -0.310353457 -3.1682825142
C 0.1862528123 -1.0582563095 -3.7509274545
C 0.4458748033 -1.6863586014 -5.0088297149
H -0.3479292589 -2.2896065909 -5.4333482849
C 1.6345820037 -1.4727272528 -5.6587697427
H 1.8228009952 -1.9321684898 -6.625099605
C 2.6226102839 -0.6449482576 -5.0753468057
H 3.5643768651 -0.4668977527 -5.5794965439
C 2.3565003403 -0.0957214941 -3.8394399556
H 5.4199239111 -1.1375358362 1.2101530702
C 5.0104950598 -0.7416086351 0.2900390948
C 3.6287886119 -0.5913958611 0.1229878291
N 3.1068219889 -0.0722824606 -1.0089439657
C 3.9283517749 0.2981044874 -2.0224994321
C 5.3201891046 0.2070127676 -1.9062232073
H 5.9656678767 0.4992655613 -2.7242574269
C 5.8528465707 -0.3228943526 -0.7358930468
H 6.9292402574 -0.4169347109 -0.6239132196
N -1.0453463421 -1.2125171148 -3.2483313422
N 3.3018527599 0.7726810394 -3.1876987411
N 2.7352593037 -0.9786711348 1.1468127838
N -0.8218655056 1.9872720309 0.2946659073
Co 1.0646450924 0.3107049805 -1.2813126701
C -1.4570393925 3.2704120723 0.6204327608
H -1.910820724 3.6663390455 -0.2897809308
H -0.6879162245 3.9688935137 0.9595216226
H -2.2338527935 3.1972755582 1.3939876378
C 4.096841605 1.6371847151 -4.0688888741
H 3.4220664622 2.0989028421 -4.7918437922
H 4.8858043871 1.1055097586 -4.6185040437
H 4.5571152163 2.4253375164 -3.4678144276
C 3.1880573381 -2.0421226346 2.054534441
H 3.6345678221 -2.8399855661 1.4579541502
H 2.3176439258 -2.4490865441 2.572724831
H 3.9200455731 -1.7057297792 2.8012078203

```

Listing S10. Coordinates of $5^{(II)}$, deprotonated.

```

H 2.4081871992 -0.277680035 3.7971316852
C 1.7250854199 0.1657679789 3.0847602301
C 0.7414626514 1.0506961359 3.5138474912
H 0.6417591985 1.2740278899 4.5720410244
C -0.1148064067 1.654557536 2.5934799083
H -0.8943767244 2.3280750807 2.9256070396
C 0.0404673176 1.3396527198 1.2448373417
N 1.0017272768 0.4821452078 0.8227826273
C 1.8412011454 -0.0975262869 1.7142396008
C -1.5744450636 1.0599398932 -0.5801021887
C -2.9630724138 1.1672990881 -0.6332324874
H -3.4927893597 1.8893426528 -0.025311088
C -3.660107314 0.294110183 -1.4675551806
H -4.7429972435 0.3523025813 -1.5270615322
C -2.9765546853 -0.6502050093 -2.2265917957
H -3.5165256026 -1.3067711852 -2.8960793767
C -1.5798269595 -0.6984580892 -2.1407287501
N -0.9049182769 0.1452385704 -1.3234855896
N 1.2204733435 -0.4698089539 -3.1144123047
C 0.2634640256 -1.2393285863 -3.6865869975
C 0.3696557758 -1.6392070606 -5.0245383679
H -0.4035586762 -2.2351502622 -5.4911800363
C 1.4688627167 -1.214336473 -5.7634157238
H 1.5639353136 -1.5071986947 -6.8049470175
C 2.44698251 -0.4125328066 -5.1758115931
H 3.3137025581 -0.0960735498 -5.7417085008
C 2.2930426333 -0.0618130346 -3.8359026865
H 5.523572702 -1.1367510869 1.1832283873
C 5.0731279459 -0.7671488268 0.2714570988
C 3.6853625895 -0.6161872536 0.1621568163
N 3.1275803742 -0.1251202053 -0.9705550231
C 3.9091769249 0.2392030531 -2.01644851
C 5.2974371058 0.1279327374 -1.9627510018
H 5.9150839125 0.4059502938 -2.8069907617
C 5.8727669857 -0.3859455789 -0.8011281799
H 6.9518685386 -0.4876179614 -0.7319055032
N -0.839183017 -1.6303562706 -2.8985633077
N 3.2404675866 0.7524791509 -3.1593133375
N 2.8312686978 -0.9757979344 1.2262393128
N -0.7864977406 1.9102529566 0.2404143712
Co 1.1236942094 0.1547001941 -1.1807163091
C -1.3528972251 3.2407229734 0.5386567914
H -1.7186303671 3.6775520621 -0.3923198494
H -0.5555393865 3.8762170634 0.9280360501
H -2.1734747975 3.2134149128 1.2660023484
C 4.0055913976 1.6980548265 -3.9960975865
H 3.3090080213 2.2137438577 -4.6594166464
H 4.7830948034 1.2161723399 -4.6013830547
H 4.4724165839 2.4378489028 -3.3433212465
C -1.5433689515 -2.8618458785 -3.3073250246
H -0.7998321592 -3.6189499477 -3.5615436258
H -2.2128538583 -2.7147760062 -4.1634944282
H -2.1236826977 -3.2278718434 -2.4589432529
C 3.3367450216 -1.994699976 2.1674001015
H 3.813207678 -2.7913087494 1.5938410085
H 2.488501697 -2.4236856745 2.7032724305
H 4.0554470653 -1.5959276216 2.8936062003

```

Listing S11. Coordinates of $\mathbf{6}^{(II)}$.


```

H 2.6399158484 -0.0726273147 3.8174226313
C 1.8775001549 0.3128221623 3.14766072
C 0.860397267 1.1377355369 3.6159524198
H 0.8000622757 1.3909550058 4.6700943631
C -0.0785263765 1.6351006735 2.7180222209
H -0.8980952898 2.2624630719 3.0542817833
C 0.0304703623 1.273671019 1.3705368515
N 1.015473605 0.4827843016 0.8925905262
C 1.9236281929 0.0218089511 1.779477405
C -1.6300858993 0.9912215543 -0.4717749545
C -3.0196187676 1.1384099007 -0.5487743018
H -3.5374577364 1.8209054792 0.1179264236
C -3.7189075638 0.3616366589 -1.4665840571
H -4.7985733478 0.4443765907 -1.5466244387
C -3.0185846764 -0.5227427639 -2.2804444134
H -3.5305810322 -1.1266278946 -3.0231586947
C -1.6267623137 -0.5885770249 -2.1515259928
N -0.9288488794 0.1484140586 -1.2604211486
N 1.2341013821 -0.5018241485 -3.1135268263
C 0.2226203404 -1.146878512 -3.7341949613
C 0.2596151171 -1.5152536161 -5.0837120756
H -0.5866292142 -2.0203456973 -5.5388288566
C 1.3843125314 -1.1822012599 -5.8313954092
H 1.4424657579 -1.4454657572 -6.8831819582
C 2.4335971035 -0.5079018421 -5.2157388973
H 3.3351864611 -0.2538685391 -5.7643499996
C 2.3209768073 -0.1980948076 -3.8556470706
H 5.5937489262 -0.9064460363 1.3000881847
C 5.1632404951 -0.6302295309 0.3426411168
C 3.7762529113 -0.5169304231 0.1956880191
N 3.1799956115 -0.1604351463 -0.9625527709
C 3.9831911581 0.1039519342 -2.0156662629
C 5.3798279365 0.0383259106 -1.9519063473
H 5.9805595581 0.247800417 -2.8314651848
C 5.9716661965 -0.3406096537 -0.7516990551
H 7.0521756193 -0.4098128884 -0.6699826434
N -0.9158588832 -1.4736172788 -2.9790216024
H -1.5428086939 -2.0756773812 -3.4991758444
N 3.3831453504 0.4748782682 -3.2298233418
H 4.0739696072 0.7814187621 -3.904271961
N 2.9575460822 -0.799857249 1.3015948217
N -0.9222976595 1.7652370282 0.4626251388
H -1.5205760056 2.4586222234 0.8955569344
Co 1.1242913003 -0.0077985716 -1.1121560554
H 3.4927483795 -1.1986261709 2.0636555656

```

Listing S12. Coordinates of $\mathbf{1}^{(1)}$.

```

H 2.8746868526 0.0977355762 3.7787933946
C 2.0341626544 0.3922608777 3.157336473
C 1.0200046961 1.2413974594 3.6413216224
H 1.0575727915 1.6032969941 4.6661715357
C -0.0103335434 1.6066459162 2.8096181318
H -0.8254981404 2.2403282344 3.139349318
C -0.0807859236 1.0952831462 1.4735737979
N 0.9467264871 0.311204857 0.9955750744
C 1.9478060501 -0.0208371805 1.8346112905
C -1.6609849206 0.8388919794 -0.3305445802
C -3.0288015795 1.1407775095 -0.625438086
H -3.5271986395 1.8373384469 0.0386043597
C -3.6813381193 0.518652045 -1.6608405276
H -4.7291700263 0.7257459887 -1.8637791759
C -2.9728666913 -0.3976153759 -2.4587864384
H -3.4440205077 -0.903608864 -3.296467349
C -1.6293687237 -0.6016507768 -2.1729748573
N -0.9496904452 -0.0108257182 -1.1653945703
N 1.1974937714 -0.5523108804 -3.1274251947
C 0.1959880941 -1.2076009983 -3.7483513554
C 0.2567058229 -1.5786750846 -5.103508195
H -0.5764135074 -2.0991146878 -5.5655532389
C 1.3764931741 -1.2113327501 -5.8388215222
H 1.4472585694 -1.4688649727 -6.892247296
C 2.4063242924 -0.5099690645 -5.220388038
H 3.3054757919 -0.2332244205 -5.7622760779
C 2.28193711 -0.2185560551 -3.8528727183
H 5.5831873511 -0.8220089355 1.315890353
C 5.1429433777 -0.5725662921 0.3547986834
C 3.7538282634 -0.5358942535 0.2225447749
N 3.1096092695 -0.2064978415 -0.9366281124
C 3.9178681219 0.0992645185 -1.9878922554
C 5.3135445081 0.087450469 -1.9358414948
H 5.8901905223 0.3209897833 -2.8266856918
C 5.944367977 -0.2586607354 -0.7430123242
H 7.0272390708 -0.2803411318 -0.6698440072
N -0.9313852662 -1.5282900998 -3.0052848127
H -1.5878248575 -2.0717895702 -3.5524030381
N 3.32180139 0.4575151813 -3.2152069231
H 4.0205176236 0.7673441814 -3.8787363571
N 2.9603588761 -0.8789655451 1.3249964856
N -1.1976126437 1.3963975266 0.797336514
Co 1.1016177713 -0.1522114278 -1.0234968577
H 3.5366532544 -1.2256480287 2.0828392866

```

Listing S13. Coordinates of **1^(f)**, deprotonated.

```

H 2.4049938529 -0.3518487334 3.7894300982
C 1.6928536356 0.1062901368 3.1094552344
C 0.6043806105 0.8200334986 3.5865937242
H 0.4289733624 0.910734889 4.65416078
C -0.2557364767 1.4310166434 2.6723625336
H -1.1157758913 1.9912582115 3.0173906919
C -0.0045110005 1.2865620779 1.3091604668
N 1.0380508776 0.5621525101 0.8203885654
C 1.8811976288 0.0140436233 1.7230484877
C -1.6244978692 1.1122054926 -0.5015076039
C -3.0171068553 1.2257450959 -0.5437249035
H -3.5389839181 1.9239449599 0.097721213
C -3.7292960301 0.3822101867 -1.3972171829
H -4.8132166802 0.4389296809 -1.4378992292
C -3.0483022458 -0.5236226684 -2.1960397287
H -3.575209018 -1.1680693759 -2.8929583335
C -1.6467146639 -0.5494324331 -2.1191938295
N -0.94933333 0.2327857743 -1.2783998753
N 1.2284235975 -0.4815385308 -3.1078838855
C 0.211774244 -1.1560810383 -3.6961115352
C 0.2567527604 -1.6193113447 -5.0173308889
H -0.5946361245 -2.1422256226 -5.4419909381
C 1.3905911671 -1.3640831464 -5.7777467055
H 1.4519839887 -1.7022818231 -6.8074972405
C 2.4474247589 -0.6695084137 -5.1969011817
H 3.3596262693 -0.4725980632 -5.7514052864
C 2.3287416329 -0.2585804933 -3.8665026312
H 5.6461609141 -0.6969541856 1.2870179062
C 5.2088021598 -0.4632097619 0.3215827821
C 3.8169132706 -0.3982334823 0.1670639685
N 3.2257353453 -0.0955256281 -1.0064349989
C 4.0164080028 0.1524974431 -2.0687479354
C 5.4156419579 0.1454010167 -1.9954201378
H 6.0160190222 0.3491135238 -2.8763438212
C 6.0081639481 -0.173741128 -0.7784002652
H 7.090169988 -0.1994106163 -0.6883820737
N -0.9501067618 -1.4247489319 -2.9574089383
H -1.5783542374 -2.0351960874 -3.4651571147
N 3.4079156326 0.4386396626 -3.2951520182
H 4.090385147 0.7008291614 -3.9960550471
N 3.010743008 -0.6824149003 1.2713156608
N -0.8505201809 1.9208794523 0.3580203338
Co 1.1379956711 0.1180325824 -1.1544223438
H 3.5461477353 -1.0655060023 2.0403029593
C -1.4287469329 3.2085286592 0.7558068704
H -1.7947534458 3.7170656893 -0.1393461327
H -0.6390251227 3.8173578359 1.2006901785
H -2.2559834044 3.1278446033 1.475479352

```

Listing S14. Coordinates of $2^{(I)}$.

```

H 2.369410015 -0.4353941286 3.7260421143
C 1.6577316008 0.0474285191 3.0627953632
C 0.5684264638 0.7406144798 3.5655607528
H 0.3939078142 0.7920735827 4.6359195817
C -0.2984147916 1.3776525091 2.6749461085
H -1.1632010785 1.9170206271 3.0407238622
C -0.046377675 1.2851650003 1.3078284016
N 1.0058022926 0.593122281 0.7935869496
C 1.8474743501 0.005889321 1.672990657
C -1.6591309468 1.1594030806 -0.5155233318
C -3.0503777502 1.2797782016 -0.5820646089
H -3.5834520351 1.9638834673 0.0651287379
C -3.7480186678 0.4610359196 -1.4713766311
H -4.8305654072 0.524810273 -1.533180145
C -3.0561464367 -0.431527691 -2.2750827701
H -3.5726758618 -1.0591825089 -2.9947146302
C -1.6557960577 -0.4677136503 -2.1707554404
N -0.9720820371 0.2985838814 -1.3032787155
N 1.2095349568 -0.3642995328 -3.1352381739
C 0.2474642415 -1.1349484828 -3.6894400398
C 0.3850726818 -1.7533213818 -4.9416397394
H -0.4229184004 -2.3565169047 -5.345008676
C 1.5531207218 -1.5510293332 -5.6588848062
H 1.6904358432 -2.0146869854 -6.6309679815
C 2.5489685111 -0.7367210288 -5.1156201043
H 3.4757867992 -0.5718204444 -5.6507818971
C 2.3408456613 -0.1626889813 -3.8631608359
H 5.597897887 -0.8684316465 1.1724154645
C 5.1643782719 -0.5567394562 0.2271976016
C 3.7743277931 -0.404666388 0.0938803944
N 3.1936411472 -0.0094919962 -1.0525468462
C 3.9823545724 0.2774873018 -2.1152641739
C 5.3758668823 0.1828415774 -2.0540322773
H 5.9892367626 0.4024130002 -2.9180376728
C 5.9624155563 -0.2497919983 -0.8638200302
H 7.042186913 -0.3446818933 -0.7937887391
N -0.9550385968 -1.3427477667 -3.0023638303
H -1.5743470736 -1.9637555263 -3.5075532754
N 3.3300333622 0.6873983283 -3.2970250458
N 2.97141879 -0.6834254754 1.2011591429
N -0.900404484 1.9425108884 0.379970102
Co 1.119474034 0.2378593724 -1.1995041785
H 3.4985556175 -1.1038022275 1.9560319044
C -1.4936628533 3.2084764637 0.8223837232
H -1.8573251407 3.7485006729 -0.0551138168
H -0.7137085392 3.8069596703 1.2973241888
H -2.3259067009 3.0914284591 1.5311776831
C 4.1074094726 1.5012009378 -4.2373005601
H 3.4192504862 1.9447738111 -4.9596656901
H 4.8780122501 0.9409795973 -4.7860904895
H 4.5922387831 2.3074442042 -3.6817175807

```

Listing S15. Coordinates of $3^{(1)}$.

```

H 2.3035168611 -0.7178060776 3.6227286606
C 1.6013690368 -0.1835619112 2.9876793262
C 0.4911780712 0.4590212521 3.5270274928
H 0.2870117303 0.4170683709 4.5924955646
C -0.3437659573 1.1758240141 2.662405151
H -1.2180681485 1.6909635577 3.0428045262
C -0.055930303 1.2091847396 1.3019773427
N 1.0044396357 0.539992573 0.7441172498
C 1.8272987057 -0.1071456888 1.6099741089
C -1.6503959919 1.252278971 -0.5295288587
C -3.0315265877 1.3977467138 -0.5380976916
H -3.5363543253 2.0405562521 0.1719111815
C -3.7652158895 0.6452423898 -1.477091955
H -4.8496249407 0.7254526205 -1.5037973387
C -3.1070537549 -0.1895382179 -2.3462564399
H -3.6269601401 -0.781709517 -3.0906902638
C -1.6788934505 -0.2664931564 -2.3293583257
N -0.9772980208 0.4551561053 -1.3913749052
N 1.1596673925 -0.2736102438 -3.1807088679
C 0.142001907 -1.0580407278 -3.6952929374
C 0.4149747079 -1.9094414431 -4.8150668843
H -0.3993538534 -2.5335779814 -5.1657384882
C 1.6394982107 -1.8844688897 -5.4334472013
H 1.8402506574 -2.5199578163 -6.2926874698
C 2.6369324138 -1.0089511467 -4.9537625336
H 3.610153108 -0.9528730856 -5.4275211703
C 2.3388577817 -0.2382195412 -3.8427677521
H 5.617827721 -0.6162097406 1.1762736079
C 5.1838205045 -0.3404222761 0.2198442274
C 3.7886551365 -0.3351751084 0.0439277688
N 3.2023153701 0.0177990929 -1.1133480528
C 3.987180796 0.3813695721 -2.158105021
C 5.3862012505 0.4485585958 -2.0470131015
H 5.9986588734 0.7335479873 -2.8923334995
C 5.9760899696 0.0717865868 -0.842027849
H 7.0576554715 0.096767614 -0.7370311368
N -1.1283548954 -1.0519181808 -3.2707513317
N 3.3328283551 0.6836441511 -3.3495861
N 2.9867881359 -0.7303240497 1.1137696846
N -0.8467528539 1.9722292103 0.4071978185
Co 1.0854246574 0.3057136659 -1.2277127876
H 3.532770228 -1.1383321588 1.861435003
C -1.4082283403 3.2100564575 0.9390009772
H -1.7595091623 3.8196721867 0.1020082739
H -0.6171421233 3.7537513898 1.4622205068
H -2.2499062177 3.0688191586 1.6361297481
C 4.0673569445 1.4375975147 -4.3618978614
H 3.3570614821 1.7707644837 -5.1209800991
H 4.8619179757 0.861181608 -4.8610943864
H 4.5181018648 2.3191201241 -3.8957679099

```

Listing S16. Coordinates of $3^{(I)}$, deprotonated.

```

H 2.4795820861 -0.2183358644 3.7995138597
C 1.7741001164 0.2158507241 3.102697064
C 0.8127579933 1.1204195191 3.5443029624
H 0.7457766821 1.375515512 4.5978515783
C -0.0622098379 1.6960972952 2.6274332779
H -0.8331722769 2.3795443555 2.9596929473
C 0.0539839824 1.342579356 1.2789908623
N 0.9846757694 0.4649289024 0.8380643076
C 1.830595473 -0.0876336262 1.7382486155
C -1.6003068413 1.026974253 -0.4983683322
C -2.9950958554 1.0735704667 -0.4571365714
H -3.508789668 1.7427232278 0.2215956782
C -3.7189317328 0.2161954292 -1.2882902633
H -4.8047122269 0.2262774088 -1.2699760575
C -3.0420639205 -0.6387692393 -2.1460259639
H -3.5774580249 -1.2883045841 -2.8320393383
C -1.6396597671 -0.6150390105 -2.1346202878
N -0.9287990935 0.174054293 -1.3085393022
N 1.226041741 -0.5121855662 -3.1271442769
C 0.2052157408 -1.1330549099 -3.7585348455
C 0.2504912184 -1.4962827433 -5.109936726
H -0.5995301412 -1.9832025053 -5.5777151638
C 1.3919221271 -1.1859620075 -5.8417541351
H 1.4562840201 -1.4470810851 -6.8937345575
C 2.4501872488 -0.5379433547 -5.2133236456
H 3.3617162755 -0.3010651907 -5.7531854282
C 2.329875052 -0.2281847375 -3.853260491
H 5.4803066823 -0.8086059426 1.4047860062
C 5.0670020104 -0.5476029573 0.4386310244
C 3.6886641937 -0.5727241654 0.2186971944
N 3.1387745031 -0.2147339427 -0.9663715146
C 3.9611652498 0.1245402069 -1.975803489
C 5.3552666731 0.1877638016 -1.8337889072
H 5.9841954739 0.463202639 -2.6749901889
C 5.9045629655 -0.1487027072 -0.6050236691
H 6.9799451152 -0.1121191844 -0.4580399379
N -0.946663178 -1.4500499924 -3.0220439466
H -1.5760843391 -2.0438346611 -3.5480328479
N 3.3982540738 0.4283663777 -3.2229221969
H 4.0991364965 0.7288303845 -3.889197662
N 2.7951377345 -0.9986989146 1.2366553672
N -0.81701207 1.8965943497 0.305518964
Co 1.1044720561 -0.0184412485 -1.1309627133
C -1.4132867561 3.1987330254 0.6208839226
H -1.8349615977 3.6178972373 -0.2952090899
H -0.6241805143 3.8662062842 0.9746735906
H -2.2045429586 3.1574199606 1.3831331072
C 3.3162474029 -1.992462637 2.1808328085
H 3.8320781963 -2.7712844675 1.6151091683
H 2.4738601075 -2.4484236389 2.7061063423
H 4.0124863395 -1.581756125 2.9261429005

```

Listing S17. Coordinates of $4^{(1)}$.

```

H 2.7559005673 0.2259398687 3.6183955239
C 1.9782495392 0.5966623832 2.9605015862
C 1.1138252012 1.6100115447 3.3766303611
H 1.1927332223 2.0320215926 4.3742692288
C 0.1234432973 2.0496075759 2.4981617311
H -0.5979006397 2.7902026854 2.819217602
C 0.0439805171 1.4923727239 1.2159481514
N 0.9203198727 0.535387674 0.7785905262
C 1.8307355673 0.0750477123 1.677043184
C -1.6543580038 0.9079914045 -0.4478524084
C -2.9926546543 0.6620211323 -0.1885082687
H -3.5121660769 1.1709804109 0.615387823
C -3.6490084048 -0.2940330635 -0.9960552356
H -4.6954358817 -0.5277020089 -0.8132689694
C -2.9682608022 -0.9104026704 -2.0171044841
H -3.4431834743 -1.6194970973 -2.6861868024
C -1.5966114849 -0.5808811944 -2.2704937983
N -0.9537981328 0.2855659829 -1.4184497065
N 1.2368461817 -0.3030808616 -3.173282085
C 0.1707401786 -0.8358460027 -3.8843258811
C 0.3345828871 -1.1519679236 -5.2679490567
H -0.5196474965 -1.5837093868 -5.7763854923
C 1.5132277983 -0.8734469464 -5.918954183
H 1.6272958743 -1.091929504 -6.9779438828
C 2.5788845795 -0.3107463198 -5.1972663453
H 3.5338353974 -0.0987986903 -5.6697143578
C 2.3871118487 -0.0695154255 -3.8406367442
H 5.3593468301 -1.3217935847 1.389963341
C 4.991884425 -0.9479750821 0.4426800456
C 3.6263205543 -0.7206487699 0.2391809695
N 3.1426224828 -0.2297003831 -0.9248085206
C 4.0014607315 0.0375093149 -1.9249790097
C 5.3931182736 -0.1281900183 -1.7861576689
H 6.05629065 0.0885570239 -2.618306761
C 5.8781407215 -0.6306707879 -0.5892506862
H 6.9455252775 -0.7859092358 -0.4553584265
N -1.0484738616 -1.0934609945 -3.3806336638
N 3.4901575038 0.4910948757 -3.1341969396
H 4.2311505045 0.7382035349 -3.7782923644
N 2.6757739108 -0.9948414074 1.2413572524
N -0.9413285937 1.8986810665 0.3086364569
Co 1.0707141546 0.0596865842 -1.1589886792
C -1.6715844857 3.1286791565 0.5940654481
H -2.238389995 3.4062460708 -0.2969018189
H -0.9571437128 3.9278595424 0.8148098841
H -2.373912797 3.0462563676 1.4392720462
C 3.0404633482 -1.986066167 2.2500416837
H 3.4265409434 -2.8761377172 1.745158786
H 2.1388226319 -2.2617453108 2.8016483248
H 3.7972330244 -1.6422296749 2.9729122846

```

Listing S18. Coordinates of $4^{(I)}$, deprotonated.

```

H 2.5282300751 -0.185650587 3.7407952699
C 1.8076229969 0.2517774837 3.0614431126
C 0.8599230755 1.1600656724 3.525653425
H 0.8214963717 1.4166821916 4.5803367474
C -0.042290966 1.733810002 2.6344791484
H -0.8062272648 2.4133407138 2.9899543651
C 0.0382437035 1.3800168246 1.2822958408
N 0.9640680713 0.5097475745 0.8212630462
C 1.826560578 -0.0537239603 1.6964681173
C -1.6228491446 1.0519753487 -0.4919050221
C -3.0184281612 1.0715956281 -0.4529440755
H -3.5464341296 1.7197064097 0.2351530547
C -3.724453347 0.2161583882 -1.3012335671
H -4.8102711021 0.2075222684 -1.2869599689
C -3.0301435337 -0.6175116886 -2.1657451187
H -3.5528739025 -1.2703900468 -2.8583732653
C -1.6279122085 -0.572052036 -2.1494762279
N -0.9332911209 0.2280371129 -1.3178854689
N 1.2198189978 -0.4144859827 -3.1400681998
C 0.2539741349 -1.1397091508 -3.7363237809
C 0.3820002933 -1.6535841562 -5.0356558877
H -0.423655668 -2.2270559054 -5.4842040823
C 1.5463150864 -1.3799044164 -5.7383052807
H 1.6794803928 -1.7614763666 -6.7462619593
C 2.5443211047 -0.6046047444 -5.1442406757
H 3.4625862523 -0.3913263208 -5.6769355764
C 2.3436140023 -0.135853092 -3.8446311156
H 5.4599466723 -0.983001156 1.2819232462
C 5.043611348 -0.6502935788 0.3394541291
C 3.6600689429 -0.5762120054 0.1490162036
N 3.1151078756 -0.1239048894 -1.0022343779
C 3.9328762655 0.2442240806 -2.0139533219
C 5.3275622206 0.1960569819 -1.8975767243
H 5.968015511 0.4712491925 -2.7256407742
C 5.8790510937 -0.2537959704 -0.7015395157
H 6.9577058632 -0.3002015815 -0.5830042049
N -0.9260563285 -1.4068510299 -3.0294648509
H -1.5437095328 -2.0250761903 -3.5404163844
N 3.3163615105 0.6828019067 -3.2110641511
N 2.7622252813 -0.983606746 1.171631875
N -0.8614544853 1.9234093173 0.331763001
Co 1.0994023308 0.0806343535 -1.1610052134
C -1.486531516 3.2054794258 0.6727474252
H -1.9309667165 3.6261958856 -0.2316115422
H -0.7106260565 3.8889954388 1.0252025535
H -2.2659717437 3.1321122239 1.4446746506
C 4.1161012208 1.5405310159 -4.0915724868
H 3.449719177 2.0074039728 -4.8196876383
H 4.9100539667 1.0076270234 -4.6341521727
H 4.5739985642 2.3285834836 -3.4892741674
C 3.2529837824 -2.0089336826 2.0982066989
H 3.725120534 -2.8047093535 1.5178393449
H 2.3994560377 -2.4323686861 2.6323697645
H 3.9780035934 -1.6372465971 2.8365057787

```

Listing S19. Coordinates of $5^{(I)}$.


```

H 2.3609597812 -0.5783352613 3.7817618001
C 1.6804081642 -0.0939583301 3.0937303195
C 0.6327509712 0.6845676696 3.5763691505
H 0.4776814319 0.7827210932 4.6468764695
C -0.2113742291 1.3412528974 2.6839566452
H -1.0434510155 1.9336728826 3.0441782822
C 0.0272183031 1.1952009434 1.3146185488
N 1.0296284337 0.427227379 0.8360617372
C 1.8500146986 -0.2044915254 1.7066015621
C -1.5427282395 1.1467067494 -0.5844144106
C -2.8931416726 1.4460544843 -0.8132792468
H -3.4015098826 2.2126233315 -0.2431094084
C -3.58536072 0.7107874761 -1.770784923
H -4.6310614961 0.9266839972 -1.9696289476
C -2.9356670713 -0.3055651516 -2.4674864134
H -3.4552777636 -0.8732965597 -3.229631299
C -1.5924146371 -0.556775438 -2.1752509266
N -0.9063632272 0.1643269668 -1.2624084249
N 1.1834352751 -0.5189617222 -3.103960684
C 0.2373936392 -1.3283581685 -3.6330624943
C 0.3701747185 -1.878571064 -4.9156136
H -0.4063522349 -2.499992721 -5.3422615427
C 1.5122994001 -1.5804906786 -5.6526831137
H 1.6404948061 -1.9973124313 -6.647418694
C 2.4861303201 -0.742331173 -5.1146601777
H 3.3892764126 -0.5181154598 -5.6690074978
C 2.2795392336 -0.2209830489 -3.8345952236
H 5.5490076945 -0.6018071402 1.2843884096
C 5.1000606257 -0.3533940428 0.3304802644
C 3.7228215078 -0.4797942457 0.1299742988
N 3.1296526686 -0.1362739466 -1.0336820803
C 3.8922161011 0.3217138289 -2.0528599621
C 5.281630356 0.4626070713 -1.9295635977
H 5.8862981355 0.8009326179 -2.7609088658
C 5.8804308176 0.1243287213 -0.7198132282
H 6.9546484366 0.2285175956 -0.5978723932
N -0.8940259728 -1.6078460367 -2.832937374
N 3.2286737241 0.665114851 -3.2529470072
N 2.8867383746 -0.9949147656 1.1598090176
N -0.7859963276 1.8725805853 0.3636707158
Co 1.1086557136 -0.017932614 -1.1412429107
C -1.3125736829 3.1771347447 0.7779305973
H -1.5906195195 3.7441813179 -0.1136967565
H -0.5214400863 3.7215689435 1.2969041451
H -2.1874570372 3.1126456496 1.4406089289
C 3.9447629434 1.5453596614 -4.1817376571
H 3.2333939023 1.9264452492 -4.9168962999
H 4.7702562972 1.0523450099 -4.7148902865
H 4.3475445659 2.3934880179 -3.6229072507
C -1.6906403104 -2.78509677 -3.1934185867
H -1.0188508946 -3.6346797576 -3.3379006938
H -2.2912436783 -2.6531771038 -4.1047745833
H -2.361795378 -3.0164861934 -2.364226859
C 3.491860547 -2.0006473018 2.0389229877
H 4.0797725968 -2.6871496276 1.4268645052
H 2.6952020937 -2.5699231228 2.5238230566
H 4.1438023858 -1.5768083336 2.8161719786

```

Listing S20. Coordinates of **6^(I)**.

```

H 2.7317606104 0.0887720401 3.8674194715
C 1.9236054418 0.4107298472 3.2157954466
C 0.8414470701 1.1401420397 3.7187788223
H 0.7738712696 1.3819019538 4.7746595471
C -0.1519256342 1.5499960622 2.8216236538
H -1.0228522739 2.1011624287 3.1663209005
C -0.0396640075 1.2006517515 1.476264632
N 1.0164868725 0.5048792819 0.9540224672
C 1.9846439694 0.1384749629 1.8483785535
C -1.6613600078 0.9326571588 -0.4377249554
C -3.0313088513 1.161944417 -0.6553935217
H -3.5696423207 1.8482466144 -0.0066779312
C -3.6857173072 0.4714979474 -1.6631834692
H -4.7473518983 0.6158486133 -1.8395253833
C -2.9416547825 -0.4336194299 -2.4382425489
H -3.401522486 -0.9906638281 -3.2490736513
C -1.5879630124 -0.5980541875 -2.1603560046
N -0.9113329739 0.081080492 -1.1968124581
N 1.2331280761 -0.5009178509 -3.0777092645
C 0.2432528087 -1.1938228125 -3.6936093337
C 0.2722041301 -1.553526159 -5.0412361039
H -0.5671364825 -2.0872819996 -5.4781686772
C 1.3757489555 -1.1828814401 -5.8158149091
H 1.4310348035 -1.4456363834 -6.8677824376
C 2.4061581178 -0.4650943874 -5.2012296469
H 3.2967809454 -0.1771739861 -5.7527524495
C 2.2944828563 -0.1515104499 -3.8461224724
H 5.6548251028 -0.9482967483 1.2083096728
C 5.1991544753 -0.6722704156 0.2607807147
C 3.8149856548 -0.427917734 0.2018583274
N 3.1635889575 -0.0642198058 -0.9422248802
C 3.9501035814 0.1058048566 -2.0373118092
C 5.3246751669 -0.1121123372 -2.0635378615
H 5.8777531846 0.0149677348 -2.9893732632
C 5.9683413589 -0.5103290848 -0.8797100012
H 7.0414768749 -0.6743192268 -0.8563367329
N -0.8596761466 -1.55861988 -2.9011069783
H -1.4926704956 -2.1513652611 -3.4253307803
N 3.322531096 0.5707244695 -3.2158910496
H 4.0176115199 0.8637057105 -3.8923537203
N 3.092109528 -0.5711526448 1.3817368003
N -1.0565621258 1.6166184066 0.6126783307
H -1.7076752298 2.2345401667 1.0787148388
Co 1.123861673 0.0116209808 -1.0378388278
H 3.6788619347 -0.8850918837 2.143298944

```

Listing S21. Coordinates of $\mathbf{1}^{(0)}$.

```

H 2.9135911753 0.2000190852 3.724948836
C 2.0552107244 0.467474056 3.1146299344
C 1.0465896707 1.3245608886 3.5929762194
H 1.0990256507 1.7192327404 4.6063958077
C 0.0004929083 1.6565363793 2.7655619544
H -0.8160630354 2.2936866719 3.0871727481
C -0.0883490509 1.1056789274 1.4447112791
N 0.9349630211 0.3112248763 0.9659303188
C 1.9538644914 0.0077630272 1.8031850312
C -1.6958190691 0.8197381388 -0.3332180601
C -3.0699963 1.106734427 -0.624972855
H -3.5792589602 1.7949631307 0.0406950281
C -3.7109408837 0.4755327256 -1.664164708
H -4.7625740796 0.6706976503 -1.8678774567
C -2.9906049682 -0.4273489218 -2.4680156183
H -3.4500549086 -0.9278371773 -3.316101643
C -1.6412747387 -0.6250299157 -2.1809466617
N -0.9835540272 -0.0254065904 -1.1614473867
N 1.1968770461 -0.4887981872 -3.0529915431
C 0.2121747625 -1.1658570073 -3.7320631219
C 0.2730128831 -1.5065940026 -5.0737646554
H -0.5735237455 -2.0146784917 -5.5324352014
C 1.421213611 -1.1850036075 -5.8294273317
H 1.5030335842 -1.4439595313 -6.8804060422
C 2.4532683469 -0.5018964992 -5.1495782666
H 3.3764077329 -0.234444212 -5.6605316933
C 2.298976429 -0.1638520949 -3.8151115425
H 5.5767560981 -0.9432688291 1.2931861736
C 5.146577712 -0.6580925192 0.3346787724
C 3.7705421276 -0.5466146206 0.2165049929
N 3.1142019751 -0.1556685124 -0.9259259145
C 3.9394756632 0.1215080054 -1.9949246639
C 5.3189739959 -0.0030988224 -1.9696990032
H 5.8860209932 0.2022361399 -2.8758365454
C 5.9715441115 -0.392924087 -0.7797599927
H 7.0521604302 -0.4782586475 -0.7222381416
N -0.9169855713 -1.5500718154 -2.9672416499
H -1.5552883796 -2.0836446121 -3.5457124869
N 3.2943202311 0.6023508904 -3.160402033
H 3.9848549351 0.9171702842 -3.8322793816
N 2.9475407087 -0.8760337625 1.3222034276
N -1.2264955362 1.3873748838 0.7898982423
Co 1.1219309828 -0.1332010214 -1.0877774698
H 3.523331252 -1.1973494403 2.0916923038

```

Listing S22. Coordinates of $\mathbf{1}^{(0)}$, deprotonated.

```

H 2.2821574854 -0.474120874 3.8155502072
C 1.5920970718 -0.0068971904 3.1168524113
C 0.4320748973 0.6195386159 3.5667081806
H 0.1820483119 0.6393938439 4.6228200242
C -0.3793123435 1.2672362917 2.6162833242
H -1.2789997505 1.7897060392 2.9215523526
C -0.0084399557 1.2427367355 1.2816592379
N 1.0809093883 0.5626851283 0.8051711334
C 1.8940433853 0.0075180479 1.7515341921
C -1.5728342528 1.1470995376 -0.5327888125
C -2.9616744768 1.2847314114 -0.5791948046
H -3.4614814072 2.0160305508 0.044800153
C -3.699242575 0.444093593 -1.417015589
H -4.7802455864 0.531545352 -1.475029412
C -3.0190676198 -0.5074438562 -2.1830513376
H -3.5481076 -1.1606415266 -2.8713790106
C -1.6291060347 -0.5806529779 -2.0762406225
N -0.8987104905 0.2218668908 -1.272018501
N 1.2458748279 -0.608969772 -3.0527011403
C 0.1716064286 -1.1936382871 -3.6570796935
C 0.1064165348 -1.5139915414 -5.0068875471
H -0.7988288035 -1.9530216764 -5.4160500286
C 1.2239823063 -1.2588184073 -5.8242485941
H 1.2161516379 -1.5154698851 -6.8788945214
C 2.3410203354 -0.6849760417 -5.2360749514
H 3.2406527259 -0.4938301468 -5.8160288513
C 2.3264769644 -0.3852739128 -3.8648283973
H 5.7029662906 -0.3795399009 1.3605632901
C 5.2651902698 -0.2532760299 0.3743294595
C 3.8772456562 -0.2891444562 0.2174206947
N 3.2526286329 -0.1285099178 -0.9874498094
C 4.0587138468 0.0626105829 -2.0688479755
C 5.4544376566 0.157692704 -1.9850476309
H 6.0424785835 0.3191736799 -2.8844488598
C 6.067673053 -0.0120297188 -0.7447317602
H 7.148210725 0.037624979 -0.6502580868
N -0.9254593105 -1.5348442853 -2.8321009036
H -1.5674744076 -2.1379923837 -3.3326387763
N 3.4828786632 0.1810779758 -3.3272594727
H 4.1736239494 0.3736149954 -4.0401329945
N 3.1029814133 -0.5592821486 1.3443015799
N -0.763272281 1.953900642 0.2967495733
Co 1.1949675117 0.0305879184 -1.1413419019
H 3.6655982838 -0.8569111225 2.1302257487
C -1.3001501507 3.2466935647 0.7018642386
H -1.6418955879 3.7793235332 -0.1910836843
H -0.4967004861 3.8213369487 1.1698521784
H -2.1419437168 3.1914364974 1.4120256911

```

Listing S23. Coordinates of $2^{(0)}$.

```

H 2.4541769195 -0.2070143952 3.8278106854
C 1.7282711692 0.2147523936 3.134935339
C 0.6499416158 1.0015118491 3.5988593001
H 0.5046463313 1.1954061231 4.6574429693
C -0.2053791551 1.5524341671 2.6259545705
H -1.0492912277 2.1669192504 2.9240680392
C 0.0279151391 1.3141753881 1.2795492516
N 1.0416125906 0.4959260338 0.8137851382
C 1.8719301358 -0.0120570804 1.7748121808
C -1.5760997471 1.0223715357 -0.5099699362
C -2.9615761062 1.0533968183 -0.4517589987
H -3.4546145473 1.7341900011 0.2352815513
C -3.72223053 0.2073932151 -1.2809956021
H -4.807862196 0.2318708653 -1.2737259294
C -3.0099141939 -0.6501798714 -2.1494216687
H -3.5320403694 -1.3014579594 -2.848159028
C -1.623943682 -0.6529280778 -2.120598627
N -0.8651505313 0.1465340259 -1.3105302574
N 1.2799027826 -0.6890637957 -3.0996346516
C 0.1856468164 -1.1530057696 -3.7465435717
C 0.1030711752 -1.3191105547 -5.1270028259
H -0.8150572244 -1.6793436302 -5.5833556165
C 1.2242838275 -0.9645739191 -5.9023416411
H 1.1943542485 -1.0670917832 -6.9858742266
C 2.3514662161 -0.4902507813 -5.2746435125
H 3.2513485905 -0.2245001789 -5.8187261842
C 2.404273135 -0.3904048314 -3.8453798786
H 5.5296884883 -0.504840219 1.4811790709
C 5.1348981224 -0.3878530901 0.4755143253
C 3.7658034879 -0.4906796071 0.2396527935
N 3.1887337971 -0.3356982883 -0.9742634107
C 4.0057681223 -0.0937523078 -2.0621548228
C 5.4152677902 0.0774628978 -1.8630366409
H 6.0133556442 0.2878423537 -2.7430897659
C 5.9713391982 -0.0853468073 -0.6165309318
H 7.0454536695 0.017032835 -0.4707441818
N -0.9176927211 -1.550489041 -2.9552277704
H -1.5708032544 -2.0871820694 -3.5137031629
N 3.6013470989 -0.0450760078 -3.3424338904
N 2.9235623267 -0.8414643859 1.3205705374
N -0.7696544344 1.9114292273 0.2596230982
Co 1.1144680748 -0.0857867885 -1.1028551979
H 3.4795029882 -1.1552549188 2.1072989806
C -1.3440997413 3.2091366114 0.5632159979
H -1.7361919461 3.6432956152 -0.3624530567
H -0.5548074097 3.8567563133 0.9590002249
H -2.1670704843 3.1909586392 1.3021309342

```

Listing S24. Coordinates of $2^{(0)}$, deprotonated.

```

H 2.3375781285 -0.5752401716 3.783302651
C 1.6785817101 -0.0357138431 3.1088529556
C 0.706976469 0.8499191929 3.5947908062
H 0.5771613207 1.0050560472 4.6612946028
C -0.0784295303 1.5398343764 2.6676793981
H -0.844867234 2.230513784 2.9999758447
C 0.12987897 1.3355313994 1.3057395173
N 1.0463165511 0.4426704897 0.8158639151
C 1.8019581483 -0.2143587235 1.7341470474
C -1.4166956684 1.1788949747 -0.4908534935
C -2.8072095249 1.272111322 -0.5129580122
H -3.3110006654 1.9975121607 0.1151980937
C -3.5387744104 0.4229124938 -1.3461741912
H -4.6215274447 0.4863979033 -1.3937878972
C -2.8383247211 -0.5017606305 -2.1301099894
H -3.3550168181 -1.1645387054 -2.8184807371
C -1.4501510188 -0.557309657 -2.0285389885
N -0.7205521233 0.2550337547 -1.2221056064
N 1.3145506481 -0.3497198889 -2.9227332633
C 0.3803834176 -1.1078403392 -3.5538786411
C 0.4767427286 -1.5068346565 -4.883713776
H -0.3237268447 -2.0900995073 -5.3302308751
C 1.60696854 -1.1352546508 -5.6246560427
H 1.7184616148 -1.4376743943 -6.6612295177
C 2.5778425074 -0.350479476 -4.9969163697
H 3.4695269803 -0.043873685 -5.531507284
C 2.3928818511 0.0397943596 -3.6726998648
H 5.3735850021 -1.450630105 1.2549791268
C 4.9974775556 -0.998105421 0.3418534142
C 3.6335834382 -0.7504023973 0.2042394948
N 3.0816566102 -0.1588818224 -0.8856466563
C 3.9420518713 0.2174120833 -1.8812599426
C 5.3132802402 -0.0273617057 -1.8310791545
H 5.944914415 0.2572617525 -2.6645346697
C 5.8594449631 -0.6430703937 -0.7028161679
H 6.9264874337 -0.8305085919 -0.6322977426
N -0.7294077545 -1.4984069622 -2.7831127199
H -1.3445888024 -2.1161153402 -3.2989392571
N 3.3269322168 0.8566795071 -2.9857738236
N 2.7463383219 -1.1252515222 1.2272406157
N -0.6141578823 2.0245305097 0.3141063789
Co 1.1851105382 0.0837229953 -1.0609621588
H 3.2194342102 -1.6264905869 1.9695830868
C -1.1558059983 3.3274370482 0.6671430647
H -1.5098602888 3.8161661392 -0.2449717763
H -0.353594475 3.9303665572 1.1017243638
H -1.9909132812 3.2942374319 1.3873469266
C 4.146144116 1.7556660263 -3.78329211
H 3.490979913 2.31993183 -4.4528769321
H 4.9133750288 1.2519632252 -4.3954980967
H 4.6504890267 2.4556258136 -3.1110155463

```

Listing S25. Coordinates of $3^{(0)}$.

```

H 2.2292668834 -0.5944273325 3.8294274486
C 1.5890523856 -0.0360407851 3.1548345032
C 0.5585799025 0.7620398097 3.6044068039
H 0.335536207 0.8349900262 4.6675269473
C -0.1918852861 1.4988076847 2.6712945107
H -1.0119149385 2.134380582 2.9853819049
C 0.1178841282 1.3591859812 1.321776777
N 1.1037196799 0.5532387421 0.8488892811
C 1.9099250091 -0.0979099953 1.766447524
C -1.4149682028 1.2019784133 -0.4937386171
C -2.7997274863 1.2987033039 -0.557954759
H -3.3139619747 2.0410387701 0.0437413947
C -3.5271592389 0.4316352898 -1.3884294932
H -4.6081645348 0.499213922 -1.4669666922
C -2.7914168156 -0.5191028726 -2.1329737429
H -3.2830523538 -1.2006984496 -2.8232027791
C -1.4120423834 -0.5777117827 -1.9841402349
N -0.6879838654 0.2507517779 -1.1821087947
N 1.3423950267 -0.3453815207 -2.8840460243
C 0.4072333348 -1.1200286994 -3.5011545185
C 0.4603608093 -1.5009332853 -4.8356823333
H -0.3509147394 -2.0923038183 -5.2538683743
C 1.5656498889 -1.106909625 -5.6242143309
H 1.6501746302 -1.3985799855 -6.6668777025
C 2.5411300455 -0.3085459105 -5.0082528952
H 3.4157763023 0.0144047566 -5.5633748522
C 2.3958387612 0.0652917635 -3.6774181885
H 5.4248092564 -1.5195366996 1.1693685913
C 5.0532883328 -1.0407119941 0.2697060243
C 3.6893320429 -0.6184279582 0.2820139435
N 3.1413390416 -0.0509467406 -0.8549145335
C 3.9679143903 0.2304694113 -1.8937630196
C 5.3205008265 -0.0980381738 -1.9220545926
H 5.9246434068 0.1254051264 -2.7937096602
C 5.8619478573 -0.7711108671 -0.8124262034
H 6.9110959034 -1.062268036 -0.8074141536
N -0.6663472794 -1.5464892398 -2.6900768421
H -1.2803183751 -2.1663727222 -3.2058336551
N 3.3461320801 0.8747167876 -3.0040135786
N 3.0401940126 -0.7541792074 1.4500299439
N -0.6255659625 2.0530642619 0.3209766959
Co 1.2304069172 0.1549610896 -1.0330706373
C -1.1885251777 3.3368661908 0.688543351
H -1.5267127266 3.8423681066 -0.2220963685
H -0.4070099575 3.9399942376 1.160951269
H -2.0456613509 3.2836765912 1.3857187772
C 4.1766676605 1.7435349356 -3.8141311638
H 3.5273746978 2.3309538786 -4.4716285006
H 4.9160914086 1.2186549817 -4.4474928303
H 4.7223118198 2.4241292798 -3.1532256192

```

Listing S26. Coordinates of $3^{(0)}$, deprotonated.

```

H 2.5027518747 -0.3130121807 3.7430133539
C 1.8054090084 0.146326001 3.0525216241
C 0.856783929 1.0694902307 3.5052588619
H 0.7867705401 1.3235897552 4.5585753029
C 0.0006091991 1.6576099801 2.5680023555
H -0.7629958346 2.3593882069 2.8818186739
C 0.1324110202 1.323633288 1.2224324594
N 1.0385730505 0.4094514482 0.7686293272
C 1.8532831884 -0.1708772731 1.6973275184
C -1.4664002158 0.974948778 -0.5167000928
C -2.8579351532 1.0016099711 -0.5045581677
H -3.3783626064 1.7224023986 0.1154124823
C -3.574189613 0.0972786465 -1.2966408293
H -4.6593133086 0.1079015143 -1.3149491725
C -2.846814423 -0.8098918026 -2.0802533286
H -3.3474443392 -1.5098409795 -2.7437056588
C -1.4591705979 -0.8028850645 -2.0059941505
N -0.7434169782 0.0545623501 -1.2304118592
N 1.2850802136 -0.4974725015 -2.9605538657
C 0.3479647147 -1.2689483023 -3.5728831641
C 0.3966783638 -1.6147870654 -4.923320928
H -0.4023038914 -2.2108597503 -5.3547135019
C 1.4703676899 -1.1731155626 -5.6988238206
H 1.5416782571 -1.432860526 -6.7505639783
C 2.4497646624 -0.3882687828 -5.0869534066
H 3.3151216986 -0.0349188383 -5.6401007071
C 2.3153119853 -0.066986178 -3.736348651
H 5.4622132294 -0.909931908 1.341823734
C 5.0441606887 -0.5692124132 0.4016359607
C 3.6667319927 -0.5992097975 0.2043766765
N 3.0654338546 -0.129726985 -0.9345711175
C 3.8964046888 0.3028315292 -1.920115063
C 5.2818234216 0.3247749584 -1.8142324873
H 5.8815240504 0.6627062941 -2.6550205735
C 5.878950268 -0.0995474211 -0.6185391199
H 6.9568693955 -0.0788094957 -0.4935324862
N -0.7042428875 -1.7252530161 -2.7625249437
H -1.3019344467 -2.3769517377 -3.2572168863
N 3.2681625172 0.74815957 -3.1034652837
H 3.9414333786 1.1185563125 -3.7639951065
N 2.776915926 -1.1114472352 1.1811523773
N -0.6896193853 1.9002440822 0.2241189725
Co 1.1619532938 -0.0424560638 -1.0978805982
C -1.288252973 3.1941950242 0.5124574657
H -1.7023126457 3.5992449853 -0.4149059753
H -0.5055900862 3.8675241804 0.8733688064
H -2.092977379 3.1649962126 1.2664762217
C 3.2958171941 -2.1157879058 2.0963638908
H 3.8100711931 -2.8842809785 1.5128105212
H 2.4542303711 -2.5761502449 2.6217512521
H 4.0003819056 -1.7244157074 2.8497570859

```

Listing S27. Coordinates of $4^{(0)}$.


```

H 2.6270555436 -0.2070031244 3.6432135095
C 1.9067389454 0.2590931204 2.9787480204
C 1.0490823374 1.2683917071 3.4447980326
H 1.0614342655 1.5849025676 4.483963427
C 0.1440231485 1.8341771034 2.5224350433
H -0.5738901931 2.5791288078 2.8467625405
C 0.1511574202 1.4016021497 1.2019943732
N 0.9931127949 0.427318011 0.7294701741
C 1.8299960232 -0.1474958523 1.6521997814
C -1.4973988878 0.9499512838 -0.4881943263
C -2.8760655343 0.8605258632 -0.3194007691
H -3.3870388693 1.5037364237 0.3880840809
C -3.5750666789 -0.1092003424 -1.0605362808
H -4.6510657197 -0.2214603771 -0.9390225363
C -2.8818883091 -0.8935009629 -1.957303739
H -3.3727629732 -1.6211464742 -2.5949404673
C -1.478323208 -0.7191636015 -2.1413096874
N -0.7825126173 0.1463641161 -1.3161666609
N 1.2635799992 -0.3752806084 -3.047835449
C 0.2784429937 -1.1028995179 -3.6968132174
C 0.5029247419 -1.5674752719 -5.0293472611
H -0.2853081646 -2.1620989556 -5.4780902626
C 1.6381679981 -1.205362443 -5.7196719228
H 1.793015564 -1.5336780824 -6.7460692307
C 2.5972133659 -0.4021091588 -5.080677831
H 3.5186646162 -0.1077599719 -5.575726439
C 2.3635987268 -0.0314747574 -3.7570995555
H 5.3524849529 -1.0247840541 1.3772550899
C 4.9739780905 -0.6452661774 0.4337097053
C 3.606503919 -0.6562867385 0.1888797913
N 3.036232831 -0.1425234651 -0.9549903175
C 3.9109981314 0.3074046872 -1.8993585244
C 5.2905933137 0.319526137 -1.7466569828
H 5.9165192323 0.6684586858 -2.5652509454
C 5.8563689857 -0.1506348525 -0.5417885908
H 6.9316707773 -0.1619500867 -0.3894077533
N -0.9294727762 -1.3764349784 -3.1783347194
N 3.3270881682 0.7666789191 -3.0974404616
H 4.0403935287 1.0754614033 -3.7476612552
N 2.664911151 -1.1709519834 1.1215183485
N -0.7432390141 1.9184566021 0.238637311
Co 1.1254252888 0.0315825294 -1.1642378485
C -1.401209194 3.175910532 0.5338640028
H -1.9090875113 3.5246788243 -0.3696325555
H -0.6416493766 3.9112611765 0.8196917807
H -2.14700956 3.1229252352 1.3485555259
C 3.1260745281 -2.1932160258 2.0361619376
H 3.6001412697 -2.9917060434 1.4554035851
H 2.2597169822 -2.6005829422 2.5678789656
H 3.8559389525 -1.8456490362 2.7925905641

```

Listing S28. Coordinates of $4^{(0)}$, deprotonated.

```

H 2.4613765925 -0.2582894766 3.6915892971
C 1.7695524843 0.2115996911 3.0026751073
C 0.8417103246 1.1560259573 3.4572096347
H 0.7862012024 1.4195901686 4.5089657274
C -0.0131506748 1.750418604 2.5229449032
H -0.7633788445 2.4658192354 2.8385110015
C 0.1041942798 1.4079730525 1.1786209143
N 0.9966490261 0.48029066 0.7219053934
C 1.802190201 -0.1151409018 1.6496796723
C -1.5033635428 1.0758450762 -0.5592947826
C -2.8958563669 1.1237594917 -0.5552698147
H -3.4103197184 1.8564785476 0.0553713292
C -3.6173575603 0.2206828197 -1.3411130859
H -4.7023407781 0.2470261794 -1.3656195712
C -2.9032186591 -0.7078854581 -2.1074719697
H -3.4122366761 -1.4101983795 -2.7616467455
C -1.5131067477 -0.718465033 -2.0309043014
N -0.7938106224 0.1427030584 -1.2652539871
N 1.2305887035 -0.4577035301 -2.9739134856
C 0.308758297 -1.2587408679 -3.568438702
C 0.3943329558 -1.6853372024 -4.8910690899
H -0.3935952517 -2.305530005 -5.3092518574
C 1.4963270365 -1.293016895 -5.6597883009
H 1.6014754922 -1.618642653 -6.6900543694
C 2.4500697325 -0.4580962629 -5.0710363936
H 3.319771884 -0.1339769759 -5.6305033416
C 2.2777786389 -0.0442463187 -3.7516445308
H 5.3844176768 -1.1376042342 1.220242731
C 4.9694855444 -0.748290813 0.2981558767
C 3.5897452134 -0.6495767664 0.1400052556
N 3.0058378321 -0.1170518925 -0.9735475107
C 3.8389304618 0.2963740064 -1.9740867025
C 5.2246948574 0.1861984961 -1.9016117093
H 5.8394588957 0.4944559933 -2.7390438567
C 5.809767262 -0.3321246154 -0.7413408865
H 6.8887221543 -0.4105882321 -0.6494725499
N -0.7735827817 -1.6629490408 -2.7659382222
H -1.3768723591 -2.3157702475 -3.251822499
N 3.188237257 0.8320665664 -3.1135126062
N 2.6927418974 -1.090743815 1.1417636907
N -0.7176146548 1.9910493003 0.1822633083
Co 1.1069575996 0.0281357993 -1.1321230528
C -1.2997516002 3.2930832266 0.4686222543
H -1.7113820227 3.7015534877 -0.4583309635
H -0.507787059 3.9576590087 0.8252117421
H -2.1022082181 3.2753735366 1.2253239627
C 3.9503012765 1.7372864599 -3.9596317306
H 3.2613309149 2.2291001508 -4.6517098013
H 4.7432831121 1.2481631247 -4.5502302468
H 4.4151514217 2.4975715142 -3.3257294805
C 3.16609606 -2.1115241149 2.0640201448
H 3.6291035234 -2.9155110825 1.4853714808
H 2.3066375196 -2.5172756558 2.6045845077
H 3.900536807 -1.749792743 2.803198213

```

Listing S29. Coordinates of $5^{(0)}$.

```

H 2.5261487346 -0.2695950212 3.6074425467
C 1.8243682021 0.2245302748 2.9438402607
C 0.9639955222 1.2270798038 3.4272655253
H 0.9603930037 1.5105586658 4.4758636563
C 0.0873405602 1.8335927265 2.5053744571
H -0.6270933567 2.578699017 2.8377669925
C 0.1203409353 1.4494720566 1.1712604022
N 0.961569585 0.4792602894 0.6841522547
C 1.7744512722 -0.1338669647 1.6029404476
C -1.5272504292 1.0848969043 -0.5398924433
C -2.9136548726 1.0695791961 -0.4122853548
H -3.412092803 1.7459005267 0.2725793491
C -3.6392138246 0.1255456515 -1.1607655649
H -4.723008531 0.0726964759 -1.0717971897
C -2.9619344083 -0.7153148779 -2.0165434136
H -3.4706291916 -1.4336602907 -2.6506310291
C -1.5452921428 -0.6208517248 -2.1597061413
N -0.8324124617 0.2386496615 -1.3419280658
N 1.1968067598 -0.3613117148 -3.0531929856
C 0.2253974455 -1.1410704936 -3.6565888989
C 0.483437673 -1.7234249821 -4.9335918427
H -0.2912290614 -2.3612068994 -5.3458523081
C 1.6352577327 -1.4177924806 -5.6251017374
H 1.8192337548 -1.8390690593 -6.6120303233
C 2.5677508584 -0.5379596841 -5.0471826299
H 3.4857803269 -0.276222062 -5.5604846745
C 2.3028712896 -0.0434350194 -3.7728484479
H 5.2908558388 -1.1257136582 1.2630819511
C 4.9104193271 -0.7207173108 0.331351478
C 3.5400897228 -0.6692872974 0.1105674412
N 2.9733733459 -0.1211131338 -1.0115817545
C 3.8449683151 0.3348809454 -1.9699453733
C 5.2260723153 0.2823021845 -1.8349012879
H 5.8633925472 0.6221452141 -2.6439322374
C 5.7915370529 -0.2435134277 -0.6560987142
H 6.868520051 -0.2946580916 -0.5239871378
N -0.9996895083 -1.353626426 -3.1457834451
N 3.2212689811 0.8413039857 -3.1349372334
N 2.6026159523 -1.1551555432 1.0621421689
N -0.742963769 2.0153262102 0.2035734937
Co 1.0714979858 0.0927597776 -1.1967505764
C -1.3556033471 3.2915651582 0.5152820214
H -1.8351100497 3.6793814046 -0.388028427
H -0.5717200921 3.9891865813 0.8283066562
H -2.1161504241 3.2523374843 1.3170979929
C 4.0043833253 1.7092025657 -3.9920765249
H 3.3389477445 2.1633220235 -4.7319476547
H 4.8241236422 1.202312737 -4.5343216834
H 4.4456730679 2.501290502 -3.3782143072
C 3.0511144049 -2.1933243375 1.9657570597
H 3.5060268112 -2.9958346123 1.3758287335
H 2.1813132302 -2.5888492461 2.5002825506
H 3.7920709557 -1.8632236647 2.7188519685

```

Listing S30. Coordinates of $5^{(0)}$, deprotonated.

```

H 2.5375642996 -0.4152877471 3.645047456
C 1.8259914406 0.0452699438 2.9700530331
C 0.8525923332 0.9261694554 3.4536621907
H 0.7790005945 1.1449847498 4.5145718913
C -0.0233319096 1.5188270705 2.5377453817
H -0.8043901299 2.1893578548 2.8760558538
C 0.1135717767 1.2325706584 1.1817059705
N 1.0427750831 0.3567831174 0.6988249903
C 1.8776645259 -0.2298988468 1.6057910731
C -1.4675159376 0.9450478756 -0.6045572063
C -2.8571405195 1.0090112382 -0.6705746486
H -3.3976603249 1.7283197544 -0.0668942782
C -3.5428672806 0.1313837042 -1.5172119869
H -4.6246208899 0.1714989133 -1.6009861845
C -2.8016150451 -0.7997644159 -2.2526493127
H -3.2946393641 -1.4817609473 -2.9352730186
C -1.4174363292 -0.8382413105 -2.1038880989
N -0.7334103803 0.0282704668 -1.3007922705
N 1.2884754074 -0.4334134903 -3.0211631862
C 0.3877337336 -1.2569139369 -3.6333876923
C 0.4396188401 -1.5574570098 -4.9922391407
H -0.3226097536 -2.1836913964 -5.4403873748
C 1.4800001536 -1.0361441388 -5.7688432148
H 1.5540487952 -1.2687385071 -6.8267873205
C 2.4220674792 -0.207187592 -5.1501680276
H 3.2544073061 0.1982140236 -5.7131819587
C 2.2838701849 0.0882699849 -3.796204866
H 5.5098998955 -1.0488375995 1.1247364121
C 5.0677654633 -0.6546943594 0.2174074892
C 3.683242226 -0.6240232075 0.0704552404
N 3.0653030678 -0.0922379649 -1.024618237
C 3.8655971703 0.4005005604 -2.0148992585
C 5.2563537612 0.3609272939 -1.9532292417
H 5.8484328687 0.7286842667 -2.782820294
C 5.8758543958 -0.1644661762 -0.8140889225
H 6.9582092236 -0.1916174392 -0.7328440205
N -0.6204043756 -1.7848192016 -2.7917598663
N 3.1843112081 0.951676364 -3.1264985531
N 2.8169213131 -1.1397528864 1.0643915469
N -0.7190586463 1.8317246093 0.2060248477
Co 1.1656408446 -0.0349810177 -1.161945957
C -1.3264791311 3.1113943743 0.5383422419
H -1.7210679262 3.558327072 -0.3782322267
H -0.5531626665 3.7685363733 0.9453091684
H -2.1469180555 3.0462362655 1.2726925532
C 3.8983785293 1.9299669015 -3.932752953
H 3.1805762731 2.4327329175 -4.5864330686
H 4.6979033134 1.5021315108 -4.5606106113
H 4.3459437895 2.6716879851 -3.2655491805
C -1.2603892644 -3.0235197667 -3.2075018641
H -0.4835143866 -3.739878785 -3.4883183093
H -1.9525318661 -2.9121620136 -4.0590232191
H -1.8209602702 -3.4271451884 -2.3600154128
C 3.3485444437 -2.1629368685 1.9515937032
H 3.8524090501 -2.9211066838 1.3459466812
H 2.51480843 -2.6328106395 2.4805023837
H 4.0650372321 -1.7857961688 2.7006708744

```

Listing S31. Coordinates of $\mathbf{6}^{(0)}$.

```

H 2.7603965466 0.0080123296 3.7128129562
C 1.9522136084 0.348034007 3.0717663072
C 0.9510674852 1.1837916244 3.5576992782
H 0.9461459428 1.4924561371 4.5991411328
C -0.0407824876 1.6187077969 2.6884412525
H -0.8507827543 2.2551595678 3.0321995673
C 0.0016832046 1.190847055 1.3524303463
N 0.9757150922 0.4000034354 0.8562243713
C 1.92921927 -0.0047598828 1.7173347356
C -1.6683671386 0.8859031659 -0.4942225468
C -3.0508983604 1.0742658721 -0.6456264975
H -3.5811010944 1.7668960041 0.0014011203
C -3.7207386245 0.3347307345 -1.6112926333
H -4.7912858112 0.4526394991 -1.752422891
C -2.9972964081 -0.5584556422 -2.3962758118
H -3.4796373611 -1.1356563369 -3.1797249467
C -1.6159867431 -0.6594320805 -2.1933136062
N -0.9448481591 0.0440416261 -1.2610847624
N 1.2688718197 -0.6061207904 -3.159794193
C 0.231585515 -1.205661616 -3.7755089826
C 0.2116301708 -1.5119118413 -5.1412596521
H -0.6634697962 -1.9768224065 -5.5859054749
C 1.3112791954 -1.1581802017 -5.9176671645
H 1.3241349963 -1.3648473374 -6.9839865096
C 2.3912532835 -0.5344414308 -5.307026248
H 3.2766106893 -0.2603009793 -5.8730230581
C 2.3340104909 -0.2916073976 -3.9258344689
H 5.5819179088 -0.7827431962 1.2985133497
C 5.165430251 -0.5634271154 0.3197095627
C 3.7786255058 -0.5341570572 0.132439741
N 3.1898357146 -0.2433394936 -1.0436305956
C 4.0054583337 0.0303233226 -2.0829425009
C 5.4052100661 0.0526619147 -1.9817881485
H 6.011820992 0.2800918503 -2.8533845206
C 5.9881562119 -0.2530980607 -0.7592435063
H 7.0685569476 -0.2488639906 -0.6468033278
N -0.8911386874 -1.5578310982 -3.0010069112
H -1.5268071186 -2.1271508173 -3.5466333332
N 3.4443953779 0.2995581732 -3.3284777056
H 4.1294812727 0.609910369 -4.0042519904
N 2.9542559003 -0.8406807132 1.2329873886
N -1.0253078249 1.6067262657 0.508685653
H -1.6282359405 2.294228863 0.9400930889
Co 1.1393755489 0.1113129119 -1.2040115696
H 3.5141503846 -1.1875057831 2.0024984479
C 1.3027532797 2.1053410953 -1.6919484774
O 2.1044072258 2.7014134104 -0.9554963973
O 0.5753360779 2.4119682376 -2.6496398678

```

Listing S32. Coordinates of $1^{(n)}$ -CO₂.

```

H 2.5582356106 -0.1786755242 3.7480821484
C 1.7937286275 0.250773879 3.1102025614
C 0.6996551513 0.9113616653 3.6147378546
H 0.5522914484 1.001722135 4.689614509
C -0.2358344698 1.4645671501 2.7238405858
H -1.1335819301 1.96538242 3.0751031668
C -0.0086941358 1.2952008345 1.3587681313
N 1.0635562157 0.673796247 0.8295034167
C 2.0137335122 0.1738674417 1.6951826412
C -1.6605317993 0.9998862265 -0.4463304008
C -3.052920375 1.0031107706 -0.4215053076
H -3.5790972096 1.6076388765 0.3117503912
C -3.7499520168 0.1880991414 -1.3372954477
H -4.8361819632 0.1698702057 -1.3560104834
C -3.0088693551 -0.5855322493 -2.2147659606
H -3.4979797945 -1.2135973345 -2.956771741
C -1.6029844998 -0.5122905444 -2.1887535983
N -0.9075330565 0.2684045363 -1.3080822669
N 1.289304961 -0.3820202504 -3.191637453
C 0.2792115341 -1.0782100455 -3.7947502497
C 0.3751881257 -1.6113274854 -5.0943224677
H -0.4755344492 -2.1404287 -5.5193490348
C 1.5263586505 -1.4024625615 -5.8351694908
H 1.6146219492 -1.7803168786 -6.8500638764
C 2.5786966222 -0.6799670222 -5.235110153
H 3.5166414243 -0.5104307776 -5.7560795177
C 2.411593544 -0.2065505623 -3.9364267962
H 5.5932529392 -1.0031078857 1.1625993577
C 5.1996623513 -0.6923661205 0.2012092139
C 3.8126784605 -0.3314547115 0.1561061311
N 3.2447661967 0.0451672858 -1.0427902782
C 4.046378801 0.1293551663 -2.1228028941
C 5.4146648964 -0.1384624754 -2.1200192649
H 5.9932946571 -0.0601366203 -3.0361446358
C 5.9929737104 -0.5688836337 -0.9140206283
H 7.0542393886 -0.8076655555 -0.869994855
N -0.9206064 -1.279517507 -3.1244323015
H -1.5568433498 -1.8436144301 -3.6708896392
N 3.4575667361 0.5206442525 -3.3478856415
H 4.1742579096 0.7271601167 -4.0326864119
N 3.1925448206 -0.361970508 1.3454287951
N -0.9728023607 1.8163652047 0.4638551763
H -1.6195743825 2.4200230825 0.9562502339
Co 1.1636112173 0.5027769897 -1.3080987815
C 1.135274929 2.5238421117 -2.0360943812
O 1.9248621106 3.1361967711 -1.3191799005
O 0.3808350464 2.7133068726 -2.9861104551

```

Listing S33. Coordinates of $1^{(f)}$ -CO₂, deprotonated.

```

H 2.3272222157 -0.3673311437 3.8020201422
C 1.6414567126 0.1141765523 3.1106513377
C 0.5163699281 0.7849223728 3.5619125325
H 0.2875952654 0.8222735804 4.6233178857
C -0.3164540621 1.4189032602 2.6364390403
H -1.2064224566 1.9437801247 2.9625807682
C 0.0002377065 1.3239852485 1.2812521416
N 1.071264175 0.6454467503 0.821853673
C 1.8933284707 0.0879370165 1.7286410055
C -1.5960441811 1.1383780865 -0.5482110873
C -2.989978636 1.2421264965 -0.5503006851
H -3.4952124622 1.9334845622 0.1124435463
C -3.7252844415 0.4000503363 -1.3851895155
H -4.810701325 0.4454030939 -1.3940168007
C -3.0512672023 -0.4920460959 -2.2044797502
H -3.5855699771 -1.1436200393 -2.8900108469
C -1.647787916 -0.512747395 -2.160548613
N -0.921969749 0.2660394454 -1.3343358007
N 1.1778925011 -0.4610970195 -3.1681566732
C 0.1918255652 -1.1834107954 -3.736452996
C 0.2923741636 -1.7465352454 -5.0188677905
H -0.5336643758 -2.3189807703 -5.4305273621
C 1.4530640799 -1.5315772906 -5.7489593764
H 1.5629223675 -1.9520626733 -6.7445214685
C 2.4759033738 -0.7719593308 -5.1855749606
H 3.4097258069 -0.6061587287 -5.7147384402
C 2.2946983578 -0.2669079039 -3.8938421634
H 5.6671918924 -0.5709471137 1.2214104763
C 5.2119830118 -0.3492913837 0.2606257949
C 3.815315946 -0.2740054774 0.1444868476
N 3.1821984649 0.0135592753 -1.0150580472
C 3.9573374113 0.2242856526 -2.0978673784
C 5.3565707611 0.1917790287 -2.0678411692
H 5.9279457652 0.3578983117 -2.9765500667
C 5.9892865882 -0.1048433169 -0.8639651273
H 7.0730245621 -0.1497472488 -0.8060159517
N -0.9913002158 -1.3810733962 -3.0316505292
H -1.6235603019 -2.0159137528 -3.4999988242
N 3.3286082855 0.5063282309 -3.3254668152
H 4.0201651537 0.7384906902 -4.0280902065
N 3.0634243365 -0.5202410525 1.2905870785
N -0.8156454871 1.9627202941 0.301602472
Co 1.1170829584 -0.0657425822 -1.1349833061
H 3.6063666866 -0.9249065477 2.0410894552
C -1.400872367 3.2419443182 0.6960125441
H -1.7689531623 3.7496063457 -0.1998725361
H -0.6169090365 3.8554595005 1.1471391266
H -2.2325843773 3.164365579 1.414206107
C 0.9575078302 -2.0600878163 -0.5976760762
O 0.1192009261 -2.2305995263 0.3015079811
O 1.7241404627 -2.787120507 -1.2475995922

```

Listing S34. Coordinates of $2^{(1)}$ -CO₂.

```

H 2.3932215969 -0.1280494574 3.855941485
C 1.6882601723 0.2756011594 3.1331466256
C 0.5951776334 1.0506860287 3.5399162204
H 0.4138952073 1.2489335284 4.5928060407
C -0.2357270381 1.5954441974 2.551767474
H -1.0884029652 2.2086112677 2.8232897601
C 0.0436880015 1.3404701069 1.2117402512
N 1.0600540368 0.526616576 0.8040864068
C 1.8841449607 0.0468022424 1.7702348814
C -1.551527707 1.0178031698 -0.5641938436
C -2.9397465745 1.0539226679 -0.463774269
H -3.4180482979 1.7468559607 0.2201913274
C -3.707009832 0.1869288986 -1.2534996917
H -4.7925938131 0.2071322479 -1.2117636718
C -3.0370881393 -0.680095277 -2.1258911977
H -3.5836797306 -1.3379573292 -2.7974871088
C -1.6416920596 -0.6727184584 -2.1472332783
N -0.8833432439 0.1278827862 -1.3546236117
N 1.2496566079 -0.6897474035 -3.1376844786
C 0.1699764747 -1.1653709685 -3.7885505547
C 0.1127781086 -1.3662448156 -5.1686843199
H -0.7934418432 -1.7433309685 -5.6347701548
C 1.2438841575 -1.0208682792 -5.9252178172
H 1.2359279492 -1.1469601869 -7.0066358018
C 2.3557619853 -0.5194382117 -5.2885290594
H 3.2617921998 -0.2568864046 -5.8233209747
C 2.3812893553 -0.3896010291 -3.8618010374
H 5.5839003726 -0.3800800474 1.4458936575
C 5.1694435115 -0.2843018736 0.4460952988
C 3.7951114476 -0.4024400998 0.2338826694
N 3.202231319 -0.2819614299 -0.9704432777
C 3.9884758897 -0.0431478578 -2.0755106319
C 5.3984607978 0.1480839183 -1.9039817976
H 5.9797090367 0.3517634435 -2.7964756125
C 5.9779501785 0.0075928488 -0.66430474
H 7.0533500273 0.1240999752 -0.5404180719
N -0.9669580684 -1.5222978849 -3.0284732369
H -1.608559871 -2.0907602971 -3.565671503
N 3.5643874406 -0.0074738766 -3.3501556807
N 2.9848073189 -0.7061327038 1.3523112698
N -0.724786781 1.9243011913 0.1621723848
Co 1.0914002259 -0.3465172632 -1.0560467256
H 3.5386502861 -1.0287873027 2.1350241481
C -1.2782970925 3.2423403443 0.4210061464
H -1.6581963892 3.6512818104 -0.5209239903
H -0.4773047321 3.8886036171 0.7945924311
H -2.1024890691 3.265368608 1.1569868155
C 0.8531150286 -2.3963056679 -0.4659669098
O -0.0486535524 -2.4370204268 0.3713034968
O 1.6299554719 -3.1467310739 -1.0438757419

```

Listing S35. Coordinates of $2^{(1)}$ -CO₂, deprotonated.


```

H 2.3520644652 -0.5242640274 3.8393641855
C 1.696445395 -0.0060962016 3.1460516567
C 0.723711961 0.8897264752 3.5942318912
H 0.5816051873 1.0686256047 4.6556708543
C -0.05215086 1.5621736234 2.6491912706
H -0.8170735922 2.2632161425 2.960832051
C 0.1560116085 1.310237199 1.2936054839
N 1.0679443141 0.4036511427 0.8451527244
C 1.8300382353 -0.2195842973 1.7745435924
C -1.4013600412 1.1415016289 -0.5104933113
C -2.7902933284 1.2639376522 -0.5210323945
H -3.2766329058 1.9937861709 0.1149740702
C -3.5419104383 0.4263414016 -1.3462838737
H -4.6246799263 0.5020294144 -1.3731525753
C -2.8717074673 -0.4999753977 -2.1475894543
H -3.4077126608 -1.1469454827 -2.835452084
C -1.4818160523 -0.5761821047 -2.0649915531
N -0.7390031615 0.2095092972 -1.2501600217
N 1.2815692003 -0.388799674 -2.937703012
C 0.3486361102 -1.1187888 -3.5931110331
C 0.4649970835 -1.488928863 -4.9325878226
H -0.3277814098 -2.0605754328 -5.4055641981
C 1.6024018497 -1.0965987454 -5.6407998649
H 1.7331955839 -1.380248984 -6.6806676199
C 2.5608195829 -0.3191337497 -4.9894747051
H 3.4561481911 0.0024864228 -5.5077991324
C 2.3623160792 0.0279319625 -3.6535529148
H 5.4276102392 -1.4390381029 1.2686394911
C 5.0295738718 -0.9962268375 0.3606454947
C 3.6595714098 -0.7625706466 0.2460360778
N 3.0887370254 -0.194825006 -0.8422599599
C 3.9185996104 0.195659742 -1.8489288946
C 5.2952806917 -0.0237270836 -1.8183529919
H 5.9113554567 0.2677291274 -2.6604617636
C 5.8627817307 -0.6361649834 -0.7002483331
H 6.9321375119 -0.8178223284 -0.6516902408
N -0.7854387732 -1.4885501351 -2.8637917935
H -1.390667209 -2.1287927656 -3.3613222215
N 3.2843216616 0.8366772809 -2.9426885902
N 2.8035797814 -1.1033749433 1.2979964803
N -0.57915478 1.9802579955 0.2836087767
Co 1.1616155173 -0.0964910367 -1.0251019381
H 3.2606655598 -1.6290359437 2.0318812661
C -1.0970015709 3.3037387476 0.6070333045
H -1.4414500961 3.7771935293 -0.3162904356
H -0.2836643214 3.9015480454 1.0271112491
H -1.9317024302 3.3018523209 1.3268304516
C 4.0874319633 1.769970145 -3.7225701034
H 3.421479843 2.3365236546 -4.3789640559
H 4.8625101187 1.2934764244 -4.344632106
H 4.5784883574 2.4642124374 -3.0353025536
C 0.8912948351 -2.2093737164 -0.5990793693
O -0.0219740125 -2.3494227215 0.1998515539
O 1.704185005 -2.8591355777 -1.2387010042

```

Listing S36. Coordinates of $3^{(I)}$ -CO₂.

```

H 2.2754181286 -0.5409027791 3.8912907883
C 1.6373769355 -0.0056224583 3.1969493354
C 0.6310154134 0.8344887403 3.6105774851
H 0.4208115017 0.9674875855 4.6703757521
C -0.1194038107 1.5386122265 2.6513268637
H -0.9180301952 2.2087560975 2.9460559825
C 0.1512861611 1.3017036381 1.3074422974
N 1.1072800712 0.4481569854 0.8768395764
C 1.9326746515 -0.1467894598 1.8074875536
C -1.4027104015 1.137810387 -0.5256455572
C -2.7859060461 1.286639754 -0.586845386
H -3.2752104784 2.0297033387 0.0332372709
C -3.5388954439 0.4589728626 -1.4277729792
H -4.619638802 0.5511406575 -1.4833414786
C -2.8462633475 -0.4917861317 -2.2023623641
H -3.3633371697 -1.1352790435 -2.9091964536
C -1.4676953455 -0.6036065736 -2.0562639453
N -0.7246174532 0.1767415662 -1.2323656794
N 1.2849284763 -0.4160367023 -2.9117045986
C 0.345799926 -1.1394500228 -3.5707348554
C 0.4129834117 -1.4554634888 -4.9236358102
H -0.3986269778 -2.0125949391 -5.38396663
C 1.5358192135 -1.0403466788 -5.665375221
H 1.6448727187 -1.2999005255 -6.7143683682
C 2.5056202693 -0.2761384147 -5.0062768565
H 3.3908589084 0.0607540487 -5.534358809
C 2.3466283057 0.0307065403 -3.6571821219
H 5.4779567828 -1.4947833099 1.2138098316
C 5.0829863823 -1.0305021483 0.3170518564
C 3.7014372 -0.671711664 0.3298623788
N 3.1276205557 -0.1498958919 -0.8103764023
C 3.9287838542 0.1818084068 -1.8476984735
C 5.2965469329 -0.0708244024 -1.8743641187
H 5.8904222177 0.184803746 -2.743625096
C 5.8694503709 -0.724137604 -0.7679758081
H 6.9297188489 -0.9708300482 -0.7709715576
N -0.7554234927 -1.5547651552 -2.8048662568
H -1.3677861487 -2.1757693529 -3.3185675062
N 3.2842107797 0.8217749112 -2.9495505141
N 3.0664073769 -0.7994973674 1.5057308826
N -0.591485169 1.9678152492 0.2860251376
Co 1.18775623 -0.1011500812 -0.9917848865
C -1.1130597483 3.2838054396 0.6126089655
H -1.4399374552 3.768325329 -0.3127873979
H -0.3108051211 3.8776327805 1.0602814989
H -1.9656744843 3.2793671094 1.3150690113
C 4.0903314547 1.7448753795 -3.7297321336
H 3.425307487 2.3302270763 -4.3724360975
H 4.8489677175 1.2633886264 -4.3723441682
H 4.6093952474 2.4220826194 -3.0451313596
C 0.9745757111 -2.1533212438 -0.5227840882
O 0.0741198222 -2.3132843401 0.2934575412
O 1.7904680264 -2.8208212742 -1.14848703

```

Listing S37. Coordinates of $3^{(I)}$ -CO₂, deprotonated.

```

H 2.5535259291 -0.2939791081 3.7102495123
C 1.8400947948 0.1664195892 3.0374007515
C 0.9115150269 1.0967797571 3.5099818471
H 0.8773913821 1.3596162444 4.5629310557
C 0.0220105443 1.6758798409 2.6012951333
H -0.7359134485 2.3746741999 2.9341641093
C 0.1090379588 1.3300911551 1.2542415919
N 1.0119259186 0.4286104244 0.7813892981
C 1.8488700255 -0.1546410119 1.6819839729
C -1.4973047625 0.9736923133 -0.4925739534
C -2.8913061755 1.0058215247 -0.5397124899
H -3.4347750473 1.7259750622 0.0600020063
C -3.5687524767 0.0958535211 -1.3529823555
H -4.6527154088 0.1067883454 -1.4138825747
C -2.8216029735 -0.8224169725 -2.0928402777
H -3.2998167117 -1.5299931587 -2.7639051805
C -1.4336425724 -0.806924618 -1.9745565097
N -0.7599266972 0.0630089255 -1.1884592939
N 1.3210677852 -0.4906434559 -2.9657452963
C 0.3782247503 -1.2717320252 -3.5406276672
C 0.3982307798 -1.6286883011 -4.8895070709
H -0.4053031981 -2.2318602143 -5.3012555386
C 1.4462990168 -1.1746761337 -5.6891318511
H 1.4893055841 -1.4319342659 -6.7431789802
C 2.4391717094 -0.3877362613 -5.1091284783
H 3.2892648998 -0.0349613279 -5.6847834618
C 2.3404180462 -0.0697759046 -3.7524186615
H 5.4386913884 -0.9273657135 1.3473130114
C 5.0347115824 -0.5806801034 0.4036337507
C 3.6587293367 -0.5972244272 0.18590388
N 3.0895648213 -0.1230607601 -0.9588184066
C 3.9271246699 0.3007688516 -1.9351400789
C 5.3128631411 0.3257678818 -1.8033914406
H 5.9289029148 0.6622753484 -2.6320155562
C 5.8808691589 -0.1036755643 -0.6003258633
H 6.9563932825 -0.0808725866 -0.4547095486
N -0.653471369 -1.7319749056 -2.7015958924
H -1.2383474359 -2.4094889704 -3.1770675874
N 3.3283308045 0.7021241797 -3.1389560858
H 3.9834566036 1.1098558598 -3.7936405544
N 2.748981031 -1.1092349275 1.1440522653
N -0.7711568116 1.8765693367 0.3009450149
Co 1.1740859614 0.0950141941 -1.116995265
C -1.3417040527 3.1919638216 0.5540504296
H -1.7371843813 3.5808152835 -0.3871747691
H -0.539288303 3.8532848714 0.8896621472
H -2.1454814756 3.1923816145 1.3082617253
C 3.2472632125 -2.1380370824 2.0474500081
H 3.7441088402 -2.9101362481 1.4538021684
H 2.3956827402 -2.5862868056 2.5665811219
H 3.9599517355 -1.7725066594 2.8048871002
C 1.2852300176 2.1780065336 -1.6474703859
O 0.5492482916 2.4013009686 -2.6002574527
O 2.0585796154 2.759277865 -0.8991033733

```

Listing S38. Coordinates of 4^(I)-CO₂.

```

H 2.6267239807 -0.2594047952 3.6102920467
C 1.9051711043 0.2240162693 2.960497802
C 1.0601750472 1.2288638616 3.4483042074
H 1.0927309177 1.5286778888 4.4921215908
C 0.1441405863 1.8170052459 2.5591049896
H -0.5660909473 2.5582211602 2.9068591946
C 0.1271419583 1.4052831526 1.2298286567
N 0.9700498912 0.4504814302 0.7362507198
C 1.8149507082 -0.1508152425 1.6238882289
C -1.5216344769 0.9710736484 -0.4682460191
C -2.9049100005 0.8849036148 -0.3399727163
H -3.4319426967 1.5284588748 0.3548158768
C -3.5793452983 -0.0938630655 -1.0893558018
H -4.6580068529 -0.2064493365 -0.9948674581
C -2.8645921312 -0.8968446678 -1.9474156832
H -3.3367217741 -1.6388631822 -2.5819001921
C -1.4557457116 -0.7170295981 -2.1039964376
N -0.79576531 0.1777143434 -1.2910822733
N 1.2909154248 -0.3619292042 -3.0587516215
C 0.3094426482 -1.1259115041 -3.654246205
C 0.5165166201 -1.6316142302 -4.9742530951
H -0.2744504224 -2.2437807253 -5.3926129799
C 1.635359599 -1.2767728267 -5.6929502159
H 1.7736166471 -1.6311425614 -6.7128645784
C 2.6021452046 -0.4545725224 -5.0956247258
H 3.5166705897 -0.1771390573 -5.6116092648
C 2.3896916813 -0.0470969125 -3.7795738286
H 5.3188740533 -0.9940428 1.3812640562
C 4.9550303191 -0.612355272 0.4333190121
C 3.5931409604 -0.6341794301 0.1573406078
N 3.0551989362 -0.1224389628 -0.995334655
C 3.9365853456 0.3266537613 -1.9285294789
C 5.3130487069 0.3594880258 -1.739677222
H 5.9565268168 0.7115662676 -2.5420696801
C 5.8467760362 -0.1014775362 -0.5213808177
H 6.9174797782 -0.0912954931 -0.3393398219
N -0.8852130192 -1.4065724999 -3.1060661944
N 3.3777883309 0.7291382584 -3.1466284335
H 4.0725902976 1.0723451618 -3.7970996659
N 2.6310292415 -1.1712978124 1.0583546916
N -0.8004590676 1.9113273892 0.3106148987
Co 1.1406160934 0.1988357489 -1.1980605857
C -1.4160702031 3.1982308593 0.5730076072
H -1.895467967 3.5438973511 -0.3457345684
H -0.6284876372 3.9086236785 0.8405809815
H -2.1688676804 3.181254872 1.3816381718
C 3.0756976865 -2.2285675504 1.9458873809
H 3.5421271523 -3.0146867462 1.3431852405
H 2.2017402017 -2.6411803562 2.4604273525
H 3.8049330776 -1.9123602897 2.7142945945
C 1.2982243005 2.2345465194 -1.6401661965
O 0.5856239485 2.5444480817 -2.5923374908
O 2.0750673042 2.7902287157 -0.8642800012

```

Listing S39. Coordinates of 4⁽¹⁾-CO₂, deprotonated.

```

H 2.4501869394 -0.1291535457 3.7055520796
C 1.7652338576 0.3131592915 2.9922973721
C 0.8158404036 1.2533835369 3.3973062975
H 0.729693282 1.5383098769 4.4416133635
C -0.0172696429 1.8252891323 2.4337653306
H -0.775886447 2.5451795065 2.7162040622
C 0.1279148456 1.4439260591 1.1011016267
N 1.030769852 0.511090973 0.6985013901
C 1.8354865231 -0.0413933394 1.645359108
C -1.4849246843 1.0833987749 -0.638511445
C -2.8770573049 1.1641838629 -0.6274064179
H -3.3739318656 1.9177339219 -0.0284294679
C -3.6178952154 0.2539986514 -1.383263893
H -4.7028777823 0.2952703678 -1.3898860595
C -2.9371293377 -0.6989460453 -2.1424609033
H -3.4675187551 -1.4003686453 -2.7793776495
C -1.5439939877 -0.7294895246 -2.0849311536
N -0.8128131062 0.1235942022 -1.3303933081
N 1.195190355 -0.5013484325 -3.0208740473
C 0.277230846 -1.2974198223 -3.6167085546
C 0.3859903293 -1.7363648347 -4.9360520497
H -0.3915273839 -2.3623049913 -5.3635001761
C 1.4957687823 -1.3405052329 -5.6840700283
H 1.6217064512 -1.6774299441 -6.708557773
C 2.4331740695 -0.4897457197 -5.095815491
H 3.3050847703 -0.1617912939 -5.6487618686
C 2.2441764133 -0.0777165373 -3.7769651712
H 5.4514520391 -1.0619179474 1.1805192415
C 5.0123794816 -0.69785779 0.2595323589
C 3.6266570222 -0.5990885105 0.1378257819
N 3.0211438585 -0.1087762493 -0.9769659829
C 3.8160298858 0.2947551984 -2.0031106459
C 5.2056075803 0.1965427617 -1.962704721
H 5.7991764526 0.4941641618 -2.818571936
C 5.8168252378 -0.3055988535 -0.8121693927
H 6.8980583665 -0.3850305465 -0.7505835837
N -0.8314934434 -1.6626521084 -2.845744607
H -1.4221835755 -2.3516785371 -3.2930703842
N 3.1370484475 0.8152044872 -3.1344696797
N 2.7743726108 -0.9821654448 1.188034582
N -0.6741990849 2.0020069901 0.0731102928
Co 1.0962446312 -0.1096669534 -1.1292825263
C -1.2295900863 3.3287749111 0.3095242222
H -1.6251271728 3.7133341447 -0.6342655214
H -0.4249760414 3.9872041545 0.6477635111
H -2.0366181028 3.3554544588 1.0595892098
C 3.8755510437 1.7391366772 -3.9862996954
H 3.1713058219 2.2191954148 -4.6708478986
H 4.6720465157 1.2671331986 -4.5841825754
H 4.3302657883 2.5065352303 -3.3541583544
C 3.223857063 -2.019099054 2.1063763126
H 3.6663631208 -2.827455372 1.5195363069
H 2.3499889883 -2.4139851331 2.6297790014
H 3.9597369038 -1.6694425215 2.8485695105
C 0.9183473652 -2.1856023764 -0.5746005893
O 0.0298814981 -2.3187984409 0.2562764073
O 1.741265577 -2.8524661985 -1.1873338177

```

Listing S40. Coordinates of $5^{(n)}$ -CO₂.

```

H 2.5488015396 -0.0987370084 3.6538422767
C 1.8433905922 0.3462337067 2.960568202
C 0.9369678338 1.3323782678 3.3824705947
H 0.8913395788 1.6463908183 4.421407573
C 0.0776958195 1.8905989865 2.4215971994
H -0.6576178981 2.6334544484 2.7091781047
C 0.1502022458 1.4578642742 1.1018281242
N 1.0157496152 0.4847185351 0.6852585824
C 1.835653677 -0.0610435408 1.6314177973
C -1.5000754996 1.0671262657 -0.626848928
C -2.8872862811 1.1315209653 -0.5425275529
H -3.3705569817 1.8548402873 0.1032001315
C -3.6382256377 0.1916331147 -1.272351597
H -4.7243848134 0.1903779542 -1.1999705676
C -2.990681642 -0.7080674688 -2.0854403827
H -3.5199288787 -1.4253165496 -2.7028778088
C -1.5682663174 -0.6800477078 -2.1999312332
N -0.8426400272 0.1582049549 -1.3807060595
N 1.1667478494 -0.4657122114 -3.0693924537
C 0.192511952 -1.2250839761 -3.6815425175
C 0.4430354037 -1.768557675 -4.9773290453
H -0.3219284811 -2.4121985595 -5.3972421657
C 1.5790310727 -1.4181811066 -5.6678106406
H 1.7624772886 -1.8097601729 -6.6668126466
C 2.5011445005 -0.5320729939 -5.0810479756
H 3.4028371577 -0.2349902908 -5.602927866
C 2.2526112016 -0.0947939373 -3.7838067779
H 5.4011998851 -1.00886518 1.2490285128
C 4.9845843269 -0.6508952075 0.3138888684
C 3.6052996661 -0.6193792109 0.1420169921
N 3.0016395077 -0.1359491008 -0.9836081523
C 3.8205540168 0.3087226978 -1.9841828129
C 5.20805756 0.2746500493 -1.8967150208
H 5.8124765201 0.5970906152 -2.7369408174
C 5.8171650102 -0.21310599 -0.7288516786
H 6.8989636345 -0.2600626107 -0.6416075734
N -1.0332428947 -1.4341318153 -3.1740138022
N 3.1560562485 0.7995155898 -3.1339854165
N 2.7209734972 -1.0506482584 1.1533776583
N -0.6857757296 1.993313894 0.092785086
Co 1.0678099999 -0.1174577723 -1.1605436508
C -1.256766863 3.3072369434 0.3345708987
H -1.6973027695 3.6741083744 -0.5966611787
H -0.4543848582 3.9864367598 0.6393590001
H -2.0383658143 3.3300987195 1.1146666085
C 3.8989402661 1.7083368381 -3.9900781819
H 3.2058259197 2.1618503987 -4.7041166603
H 4.7165424479 1.234266243 -4.5617896704
H 4.3340789269 2.4966267508 -3.3678784146
C 3.1624465147 -2.0838559899 2.0657225408
H 3.6058119428 -2.8924557363 1.4775901336
H 2.285592646 -2.4726227599 2.5912243483
H 3.9025612255 -1.7447287547 2.8148661273
C 0.849819746 -2.1522237241 -0.6668707379
O -0.0482568222 -2.3050580953 0.1558159143
O 1.6613213727 -2.8372630478 -1.2823812877

```

Listing S41. Coordinates of $5^{(I)}$ -CO₂, deprotonated.

H 2.5562759232	-0.4265279911	3.6105412514	
C 1.8361605199	0.0436734904	2.951926511	
C 0.8866555948	0.9355998929	3.4547398329	0 0.5302012804 2.4751605067 -2.5700562623
H 0.8444916422	1.1554863437	4.5173451262	0 2.0487167054 2.7617333057 -0.8676442895
C -0.0117998117	1.5334753085	2.5694377871	
H -0.784344009	2.202879977	2.9281800654	
C 0.0854660807	1.243423999	1.2084713087	
N 1.0095448944	0.3805096535	0.709281246	
C 1.856815615	-0.2219672774	1.5835309426	
C -1.5010117569	0.9503441755	-0.5807160473	
C -2.8910564854	1.0056857046	-0.6832629728	
H -3.4514240947	1.7182891655	-0.0902089347	
C -3.5417707682	0.1206144987	-1.5443718651	
H -4.6214584762	0.1521139073	-1.6564244586	
C -2.7818383395	-0.8116597437	-2.2537533986	
H -3.255585963	-1.503726265	-2.9393766301	
C -1.3986913606	-0.8290841381	-2.0802755798	
N -0.7523269221	0.0510927584	-1.272621514	
N 1.3235332474	-0.4188072489	-3.0392274647	
C 0.4099751422	-1.2430442356	-3.61509234	
C 0.4295900406	-1.5508739362	-4.9746452011	
H -0.3413283849	-2.1792724827	-5.4037578363	
C 1.4456821397	-1.0237226296	-5.7742226641	
H 1.4879506256	-1.2525594514	-6.8349306038	
C 2.4098682752	-0.2038152427	-5.1855127758	
H 3.2323550941	0.1943208157	-5.767424862	
C 2.3118033788	0.0855037402	-3.824439523	
H 5.4696143866	-1.06284838	1.1366882153	
C 5.0475759074	-0.6627593793	0.2227907954	
C 3.6654940121	-0.6228566049	0.0451045169	
N 3.086005306	-0.0843398629	-1.0590117418	
C 3.8990005209	0.3927369682	-2.0382426038	
C 5.2901321201	0.3594827756	-1.940091572	
H 5.901317456	0.7229999869	-2.7573298812	
C 5.8747108558	-0.1634125102	-0.7853733486	
H 6.9547835989	-0.1872279499	-0.6751585207	
N -0.5753951409	-1.7724546086	-2.7448758857	
N 3.2592692513	0.9023957106	-3.1818517843	
N 2.7732037309	-1.1422952463	1.0163477267	
N -0.7973910175	1.8154654664	0.2754349413	
Co 1.1728625443	0.1129063717	-1.1928700943	
C -1.3718162063	3.120802916	0.5709463274	
H -1.7406350246	3.5518830611	-0.3626924239	
H -0.5778361332	3.7650552432	0.9557121959	
H -2.1953120068	3.0895199038	1.3026928557	
C 3.9442967942	1.9207322355	-3.9659480322	
H 3.2055148251	2.423920491	-4.5939376691	
H 4.7487279415	1.5232699112	-4.6058511752	
H 4.3671590231	2.6563665525	-3.2777446378	
C -1.1947803054	-3.0333513891	-3.1340151693	
H -0.4058230436	-3.7393032203	-3.4065143086	
H -1.8940537276	-2.9514116985	-3.9818685744	
H -1.7413637775	-3.4319106186	-2.2753095542	
C 3.2811532728	-2.1950463203	1.887252227	
H 3.7705232583	-2.9520885169	1.2687577973	
H 2.4358603306	-2.6570255849	2.4041458536	
H 4.0024694584	-1.8479306662	2.6448106102	
C 1.2699419616	2.201958362	-1.6313459333	

Listing S42. Coordinates of $6^{(1)}$ -CO₂.

```

H 2.741066364 -0.2738954067 3.8090599281
C 2.0204486208 0.1809484147 3.1373069656
C 1.0859185263 1.1042249571 3.5984390142
H 1.0505865519 1.3721137007 4.6499614634
C 0.1969844058 1.6738519443 2.6973192451
H -0.5657299226 2.3736938917 3.0229066236
C 0.2660353525 1.2896702173 1.3537565829
N 1.1923291832 0.425787406 0.8807586943
C 2.0486995902 -0.1164416999 1.7742649346
C -1.352188275 0.9701718301 -0.4531923662
C -2.7384626773 1.1008291306 -0.5867745689
H -3.2708824309 1.852285564 -0.012987151
C -3.4107241963 0.2235607074 -1.426419646
H -4.4878895063 0.2914914474 -1.5438817173
C -2.6864878051 -0.7456894324 -2.1149564235
H -3.1751322541 -1.4365655634 -2.7941168693
C -1.3004686417 -0.7802536458 -1.957249051
N -0.6279119922 0.0598925906 -1.1413757837
N 1.4774504705 -0.5343479153 -2.9255286337
C 0.5202527649 -1.295507502 -3.4988451789
C 0.5391759087 -1.6605525856 -4.8455277106
H -0.2627823087 -2.2643830923 -5.2574551915
C 1.5740016466 -1.1891660317 -5.6485453196
H 1.6062038189 -1.4365743372 -6.7051610583
C 2.5651467005 -0.4007054477 -5.0805947653
H 3.4023576031 -0.0372803561 -5.6674540086
C 2.4942096885 -0.1178675594 -3.7124593645
H 5.6603163451 -1.0993827112 1.3369942084
C 5.2514833179 -0.7338280703 0.4007195985
C 3.8700875691 -0.6329105199 0.2312427877
N 3.2951449378 -0.1715325539 -0.9009602373
C 4.117077153 0.1981187112 -1.9089579836
C 5.5120484359 0.1683356305 -1.8052281189
H 6.1254869191 0.4788617523 -2.644730994
C 6.0818168962 -0.3106197234 -0.6336200772
H 7.1611575608 -0.357980562 -0.5263317859
N -0.5418057575 -1.7135288344 -2.6814224426
H -1.1311071259 -2.3911154565 -3.1514805009
N 3.5308320714 0.5910606716 -3.1090726066
H 4.1920294207 0.975519648 -3.7726415961
N 3.0133610814 -1.0072411577 1.2782739653
N -0.6758559384 1.7825797917 0.4544599992
H -1.2537098463 2.5187663775 0.8410682529
Co 1.3460532837 0.1031234303 -1.0604088795
H 3.5162147682 -1.4700351363 2.0267953148
C 1.4471838123 2.0848795087 -1.6017132808
O 0.8304089199 2.6205636898 -2.5121734446
O 2.3075128518 2.8762574485 -0.8458254551
H 2.2563061376 3.7870468387 -1.2111453675

```

Listing S43. Coordinates of $\text{I}^{(\text{II})}\text{-CO}_2\text{H}$.


```

H 2.7124292424 -0.3255867195 3.718592426
C 1.99529745 0.1586065049 3.0633943672
C 1.0988171876 1.1121331981 3.5460409926
H 1.0888419514 1.3732156665 4.6003885914
C 0.216338635 1.7144681286 2.6641155818
H -0.5200816652 2.4361875531 3.003184288
C 0.2460249901 1.3335188152 1.3128382683
N 1.1421826881 0.4470525086 0.8195588927
C 1.988323362 -0.1282017688 1.6978608368
C -1.3909954736 0.9931724914 -0.4547374688
C -2.7781717395 1.0182726796 -0.4118540771
H -3.2939445314 1.6965751824 0.2606468106
C -3.475666918 0.0944688742 -1.2075552157
H -4.5620043771 0.0634274652 -1.1831836005
C -2.7670015628 -0.7656044044 -2.0109225746
H -3.2494972082 -1.4816517467 -2.6655402543
C -1.3437019087 -0.6803911242 -2.0929031702
N -0.6645015139 0.17909256 -1.2516543769
N 1.4156152144 -0.4102878348 -3.0135051006
C 0.4297384213 -1.1855410054 -3.5923019551
C 0.6433846118 -1.7394416208 -4.8913207006
H -0.1427958863 -2.3725176105 -5.2852757286
C 1.7509353426 -1.3936435395 -5.6269128472
H 1.8884540369 -1.7746655662 -6.6356889119
C 2.7102763285 -0.5391874358 -5.0587380396
H 3.614938451 -0.2624749649 -5.5910279258
C 2.5040669725 -0.1097027543 -3.7550016315
H 5.5620690794 -1.1357132115 1.2999885855
C 5.1771140685 -0.7433706399 0.3640980868
C 3.8004350122 -0.6408408874 0.1605430419
N 3.2482106206 -0.1466052682 -0.9660181432
C 4.0923804652 0.2477116208 -1.9481710798
C 5.4892298691 0.22434286 -1.8063795293
H 6.1185228006 0.5604406243 -2.6243838423
C 6.0322832999 -0.2843553967 -0.6376473434
H 7.1093900254 -0.3319215508 -0.505324527
N -0.7744036895 -1.4182040523 -3.0546943826
N 3.5232872934 0.6544685797 -3.1379400894
H 4.2017585634 0.9973286725 -3.8063999992
N 2.9180521883 -1.0479915685 1.1783286025
N -0.6840834061 1.8425140704 0.4294465038
H -1.2820398766 2.5463706424 0.843808041
Co 1.2937283318 0.2118559041 -1.1576764018
H 3.4139166432 -1.5257052108 1.9218645911
C 1.5394209457 2.2262123741 -1.5370744339
O 1.0045738557 2.9075857161 -2.3990705956
O 2.4459632882 2.8930123514 -0.6852623416
H 2.4582585206 3.8289008381 -0.9839722201

```

Listing S44. Coordinates of $1^{(II)}$ -CO₂H, deprotonated.

```

H 2.4314566587 -0.2226437942 3.719660369
C 1.7398654485 0.2394701216 3.02254629
C 0.7614994715 1.1222071567 3.4516533939
H 0.6469725632 1.3447733864 4.5082310821
C -0.0678913057 1.7329532521 2.5111355569
H -0.8400838779 2.4233072247 2.8246284831
C 0.084606715 1.4044430963 1.1640390576
N 1.0210773044 0.5233808436 0.733245747
C 1.8540697298 -0.0120709616 1.6501587831
C -1.5348513452 1.0731465588 -0.5838976367
C -2.9276905296 1.1505379757 -0.5784311391
H -3.4343895988 1.8971572474 0.0189154397
C -3.6572279834 0.2215101535 -1.3199316127
H -4.7427094703 0.2479866506 -1.313941131
C -2.9825715409 -0.7263466842 -2.0728424035
H -3.5141973431 -1.4387712741 -2.6954455641
C -1.5827786332 -0.7184418226 -2.0541147239
N -0.8625469218 0.1353157915 -1.2963812354
N 1.1486972607 -0.4428763928 -3.0694024855
C 0.2084462474 -1.2206765864 -3.6503288466
C 0.2762422745 -1.6260587253 -4.9876419132
H -0.5043258458 -2.253543493 -5.4052667552
C 1.3319156571 -1.1729241188 -5.7667183178
H 1.4077579386 -1.4613792314 -6.8106318449
C 2.292560807 -0.3439530941 -5.1935483192
H 3.1425371413 0.0123581997 -5.7662436629
C 2.1722696389 -0.0196011669 -3.8417136217
H 5.5256550693 -0.9695594548 1.0919302453
C 5.0696167884 -0.6049888989 0.1773522323
C 3.6783537872 -0.4908014985 0.0857197437
N 3.048696761 -0.0445630606 -1.0240336533
C 3.8173500993 0.3324028169 -2.0683382852
C 5.2119850204 0.2883030621 -2.0438350268
H 5.7825693073 0.5923204577 -2.9152775684
C 5.84213362 -0.2017769223 -0.9033163739
H 6.9249288194 -0.268037318 -0.8597946639
N -0.8869499279 -1.5993876452 -2.8779443092
H -1.4798947887 -2.2846214722 -3.3295417636
N 3.1561215229 0.7713790559 -3.2264069046
H 3.803896469 1.1570471318 -3.9038512688
N 2.8932400658 -0.8164874846 1.1895890821
N -0.7504841061 1.9695010694 0.1748370267
Co 1.0810884751 -0.1064605652 -1.1278949283
H 3.4110389798 -1.2712639742 1.93137253
C -1.3292252873 3.285855464 0.4616695411
H -1.7262674807 3.6988336029 -0.4680695616
H -0.5336373355 3.9425827207 0.8199470106
H -2.1336469074 3.2666912137 1.2102385344
C 1.0095740637 -2.1152748848 -0.6777332861
O 1.705471511 -2.9938607773 -1.1677014874
O 0.0704250594 -2.4890945608 0.2794433557
H 0.1464299534 -3.462228391 0.3927567902

```

Listing S45. Coordinates of 2^(II)-CO₂H.

```

H 2.3820753367 -0.2949675755 3.7341395069
C 1.7169651036 0.1791834839 3.0190636161
C 0.7450161166 1.0794691388 3.4190550861
H 0.6060702737 1.3081819094 4.4719780986
C -0.0461734886 1.7057912884 2.4527909074
H -0.813188082 2.413587642 2.7400802285
C 0.1409743783 1.3669169882 1.1128260624
N 1.0661213892 0.4667210942 0.7068958957
C 1.871453669 -0.0765032088 1.6467193212
C -1.4721599567 1.0354169251 -0.6288600929
C -2.8633092219 1.1297954435 -0.5925199116
H -3.3481976284 1.8979619803 -0.0039125433
C -3.6176682469 0.1863800488 -1.2943045767
H -4.7030787752 0.2235351742 -1.2665821653
C -2.9676440532 -0.7835139483 -2.0372396418
H -3.5160897732 -1.5071226719 -2.6323194957
C -1.5632834727 -0.7859210137 -2.056103053
N -0.8205656233 0.0758782857 -1.3261476094
N 1.2075782431 -0.5838259972 -3.071999829
C 0.196602734 -1.2431180128 -3.6786131075
C 0.1289758931 -1.4897694779 -5.0431841408
H -0.7194091011 -2.0204396135 -5.4638569676
C 1.1524656105 -0.9716352072 -5.8539364903
H 1.1235459967 -1.1204596348 -6.9304119313
C 2.184646013 -0.2772314765 -5.2700227921
H 3.0146871218 0.1211361421 -5.841437015
C 2.2570059831 -0.137689238 -3.850753451
H 5.5164099387 -0.7019576629 1.2560084335
C 5.0824157572 -0.4411363741 0.295816867
C 3.7088474578 -0.5053542575 0.1049730741
N 3.0838152763 -0.1906890114 -1.0506129408
C 3.8566657545 0.2024146352 -2.1254127698
C 5.2623445668 0.3825085975 -1.9485110299
H 5.8211854879 0.7286702564 -2.8099253604
C 5.8697049792 0.0346976659 -0.7659631301
H 6.9466166793 0.1252132253 -0.6482350075
N -0.8827842184 -1.6698493003 -2.8693552177
H -1.490758413 -2.3209941488 -3.3497815977
N 3.4001390489 0.3727673165 -3.3732904948
N 2.8998047663 -0.883420379 1.2027959023
N -0.6594089387 1.9398585567 0.0954146523
Co 1.1305345839 -0.2476331096 -1.1456409795
H 3.4379899575 -1.295489629 1.9544659077
C -1.2064765604 3.2703089686 0.3490454464
H -1.5907601754 3.6714321502 -0.5919079387
H -0.3971918835 3.9163104854 0.6978994599
H -2.0164122815 3.2927562718 1.0943794492
C 0.9101489457 -2.2168807577 -0.5611986739
O 1.526466575 -3.1966503444 -0.9528587991
O -0.081199902 -2.4494529796 0.4150549627
H -0.0682038414 -3.4164486434 0.5882358762

```

Listing S46. Coordinates of $2^{(III)}$ -CO₂H, deprotonated.

```

H 2.4106132319 -0.1633123277 3.7949790524
C 1.7320633629 0.2957827767 3.0832166082
C 0.7580131008 1.194585401 3.4884759779
H 0.6351144064 1.4341377527 4.5404016026
C -0.0579732545 1.7978582388 2.5313337703
H -0.8285071279 2.4974889147 2.8278766444
C 0.1061485403 1.4494137951 1.1905130629
N 1.0418950754 0.5566793218 0.7834665831
C 1.8574216591 0.021307192 1.7160573588
C -1.4861672439 1.1068234587 -0.5855260106
C -2.8782839779 1.1918417812 -0.6145082733
H -3.3957641907 1.9455257117 -0.0355698596
C -3.5942911831 0.2608490546 -1.3670114142
H -4.6793832133 0.2943680667 -1.3889393438
C -2.9076298973 -0.6992645145 -2.0932383073
H -3.4288686974 -1.4151258606 -2.7206369954
C -1.5086238521 -0.7017124697 -2.0382016481
N -0.8035439878 0.1593801435 -1.2745636879
N 1.2419170143 -0.4527155715 -2.9929211664
C 0.3280303513 -1.2604264744 -3.5693714017
C 0.4482567497 -1.729159922 -4.8829076776
H -0.3106814207 -2.3837587937 -5.2991561738
C 1.5295439628 -1.303424622 -5.6379159531
H 1.6532232186 -1.6448129689 -6.6612185211
C 2.4551704934 -0.4255939804 -5.0739473458
H 3.3110102738 -0.0878766169 -5.6436250756
C 2.2860050577 -0.0305527022 -3.7468280981
H 5.5060773551 -1.1067621187 1.1885252304
C 5.0724914587 -0.7133696317 0.2747864143
C 3.6883856313 -0.5288450668 0.1766088891
N 3.0894915008 -0.0508794604 -0.9337726739
C 3.875907777 0.320495776 -1.9733614581
C 5.2652187547 0.1997460173 -1.9372166221
H 5.8650574871 0.4857541308 -2.7912592782
C 5.864237856 -0.3432685323 -0.8007556801
H 6.9418752839 -0.4693890535 -0.7584601588
N -0.7980352938 -1.6044804376 -2.8247517688
H -1.3821700922 -2.2987596694 -3.2738677731
N 3.2143068959 0.8270243442 -3.1143392319
N 2.8843580574 -0.8113567632 1.2790902923
N -0.7140561748 2.0059260512 0.183626549
Co 1.1312832333 -0.0846553618 -1.0676520282
H 3.3797992331 -1.272461731 2.0320489227
C -1.2951990603 3.3253958567 0.4500862762
H -1.6762381381 3.7317118932 -0.4892414528
H -0.5048792558 3.9840397141 0.8164686521
H -2.1119795806 3.313081165 1.1853245435
C 3.9719610869 1.7409396544 -3.9747518181
H 3.2735090044 2.2366189313 -4.6522584303
H 4.7520003809 1.2486091189 -4.5722663682
H 4.4408957889 2.5000036612 -3.3450012258
C 1.0276147715 -2.0902722681 -0.5884425994
O 0.0606977588 -2.435649355 0.3520909168
O 1.722675847 -2.9867447624 -1.0460556801
H 0.1216439809 -3.4074968869 0.4836038542

```

Listing S47. Coordinates of $3^{(II)}$ -CO₂H.

```

H 2.3389210936 -0.1984873188 3.815484131
C 1.6687937129 0.2803926414 3.1110021599
C 0.6377744235 1.094880222 3.5069174566
H 0.439948649 1.2651684686 4.5623736948
C -0.1618840258 1.7246284137 2.5326715886
H -0.9805299174 2.3730063876 2.8183132284
C 0.0979695982 1.4459116188 1.1995792367
N 1.0875520946 0.6232893203 0.7856984333
C 1.9492148034 0.0933029305 1.7242223421
C -1.4790825774 1.1324497113 -0.5929108709
C -2.8737171666 1.2277617142 -0.6598613521
H -3.3959876986 1.9927962669 -0.1000338207
C -3.5799273276 0.2894355253 -1.4090439001
H -4.6646726539 0.3286138089 -1.4544069282
C -2.8828783036 -0.6905576918 -2.1012211647
H -3.3925745194 -1.4149300022 -2.7289027899
C -1.4852793708 -0.700163919 -2.0123528305
N -0.787624852 0.1676069226 -1.2528084213
N 1.2606349908 -0.4503832324 -2.974851413
C 0.348342708 -1.2671505445 -3.5360148226
C 0.4427001493 -1.7313231218 -4.8538652966
H -0.319791983 -2.3928120607 -5.253285947
C 1.502420912 -1.2899005238 -5.6326308379
H 1.6085845262 -1.628682602 -6.6593618182
C 2.4280779284 -0.4038881575 -5.0857707267
H 3.2721975785 -0.0580631211 -5.6683282963
C 2.286826378 -0.0155625787 -3.7490481873
H 5.5334381377 -1.1229210485 1.1450921587
C 5.1097063976 -0.7217053844 0.2318602202
C 3.7148579409 -0.4232350416 0.2445667631
N 3.110837807 0.0254999027 -0.911852507
C 3.8849485279 0.3203883971 -1.980223547
C 5.2574694914 0.1249676999 -2.0110295267
H 5.8340835261 0.3538398206 -2.8981880378
C 5.8703147818 -0.4376515649 -0.8746742476
H 6.9391408505 -0.636727064 -0.8783787999
N -0.7644313919 -1.6197904631 -2.7724411396
H -1.3464996375 -2.3191024591 -3.214971544
N 3.2063536887 0.8423862876 -3.1294947994
N 3.093682477 -0.5356623528 1.4272663931
N -0.7157433568 2.0247210722 0.1710752681
Co 1.1663258694 -0.0457432024 -1.041797044
C -1.2999841963 3.3324611568 0.4536113762
H -1.6692176947 3.7623601196 -0.4817188258
H -0.5148317378 3.979630214 0.8506050098
H -2.1284089492 3.3104845114 1.1786009185
C 3.9691315406 1.7386032662 -3.9934526167
H 3.2768077252 2.2475761611 -4.6698368846
H 4.7410751406 1.2370515936 -4.5975365795
H 4.4583002765 2.4862516368 -3.3651661313
C 1.0511600901 -2.0654769078 -0.5705541981
O 0.1255949073 -2.4059644975 0.4190373803
O 1.7059723956 -2.9820008043 -1.0540863499
H 0.2257662416 -3.3718501271 0.5691044437

```

Listing S48. Coordinates of $3^{(II)}$ -CO₂H, deprotonated.

```

H 2.4409314648 -0.4352822971 3.7411158875
C 1.7594383057 0.059671043 3.0616418523
C 0.870412266 1.0256620581 3.5256670278
H 0.8382719564 1.2764812496 4.5817822898
C 0.0204682959 1.65985245 2.6307943653
H -0.7031581117 2.3868387621 2.9755720849
C 0.0796230984 1.303015746 1.27794366
N 0.9669785004 0.3926135955 0.8116791732
C 1.7873257195 -0.2225795913 1.6950313905
C -1.5319384254 0.9937421113 -0.4928308288
C -2.9276259486 1.0582385815 -0.5668440256
H -3.4729433282 1.7758508055 0.0325527162
C -3.6016030715 0.1547352838 -1.3811295365
H -4.6855726833 0.175238446 -1.4415513288
C -2.8743960656 -0.7739214694 -2.1165257089
H -3.3649328369 -1.475401935 -2.7836724183
C -1.4816043841 -0.7580097043 -2.013670742
N -0.8122917481 0.0948269411 -1.2115538888
N 1.2961903812 -0.4613161298 -2.9904594992
C 0.3449675811 -1.211548603 -3.5870152338
C 0.3823008954 -1.5510505504 -4.9402316784
H -0.414805464 -2.1442548498 -5.376383987
C 1.4350874666 -1.0734505705 -5.7166734855
H 1.483798391 -1.3049533775 -6.7763015668
C 2.4243205133 -0.3025073102 -5.1204303657
H 3.275024633 0.0606243076 -5.6878075677
C 2.3312975627 -0.0379620541 -3.7497459757
H 5.3919441276 -1.134698843 1.3286913906
C 4.9917519769 -0.738200491 0.4046506872
C 3.6137217439 -0.6832101006 0.1944301967
N 3.0756116174 -0.1673225381 -0.9371804343
C 3.9137191738 0.2617133424 -1.902675367
C 5.3049404491 0.2744872392 -1.7505736728
H 5.9379932726 0.6392883121 -2.5530059873
C 5.8428383677 -0.2298922551 -0.5766440404
H 6.9179844176 -0.2385191282 -0.4249883238
N -0.721887333 -1.649868955 -2.787336868
H -1.3070593086 -2.3193012223 -3.2735654398
N 3.3531433967 0.6641466222 -3.1142995553
N 2.7028695121 -1.1591581323 1.1633555884
N -0.8252467051 1.8508549275 0.3597577914
Co 1.1447084961 0.1234402764 -1.1216608171
C -1.3952073192 3.170013293 0.647321702
H -1.7980658858 3.5791077856 -0.2808574513
H -0.5893921879 3.8246661235 0.985041492
H -2.1897680817 3.1484643886 1.4058293425
C 3.1779600808 -2.2156779888 2.0620526741
H 3.6597762697 -2.9899617809 1.4612248102
H 2.3144853561 -2.6562771413 2.5649985464
H 3.8896346488 -1.8679485002 2.8240073779
C 1.3471094057 2.135710042 -1.516912716
O 0.6079336019 2.6125511131 -2.5986112262
O 2.0287069202 2.9426689935 -0.8985332021
H 4.0252423529 1.0682246487 -3.7548240108
H 0.8030266697 3.5723870304 -2.6777050972

```

Listing S49. Coordinates of 4^(II)-CO₂H.

```

H 2.4592914026 -0.3724598964 3.6634379738
C 1.7755440937 0.1346983136 2.9946335998
C 0.9488296225 1.1579943373 3.4581280959
H 0.9691929048 1.4441922382 4.5061535894
C 0.0908926315 1.7969321269 2.5769578224
H -0.5902478304 2.5637061953 2.9228154438
C 0.0735888407 1.3868502242 1.2333806426
N 0.9222010106 0.4382554902 0.7618617442
C 1.7384128982 -0.1850173363 1.6366198204
C -1.5596669841 0.9639726155 -0.4759470048
C -2.9376204717 0.8681543769 -0.3442710785
H -3.4715226508 1.5044142118 0.3509891228
C -3.6057788971 -0.1176680491 -1.0939434493
H -4.6810983927 -0.2417592571 -0.991584397
C -2.889586985 -0.9108900352 -1.9563319126
H -3.3574180049 -1.6592306574 -2.5855449174
C -1.4854093765 -0.7112405195 -2.1274227766
N -0.8299652242 0.18524529 -1.3093247167
N 1.2612434587 -0.3361011024 -3.0657345765
C 0.2736527116 -1.0742655891 -3.6873076157
C 0.4761550573 -1.5262275209 -5.0258778656
H -0.3143596836 -2.1243242771 -5.4634906831
C 1.5886781481 -1.1407713388 -5.7357337052
H 1.7204126045 -1.4497688241 -6.769675652
C 2.5626393559 -0.3468826575 -5.1087532235
H 3.4733111703 -0.0505461016 -5.61992475
C 2.3587721867 -0.0023293513 -3.7789838998
H 5.2840134214 -1.2591326093 1.3082909428
C 4.916330598 -0.8243892898 0.3877286872
C 3.5454193898 -0.716685514 0.1509339294
N 3.0408533925 -0.1580608016 -0.9736186982
C 3.910558298 0.2692625832 -1.9145259815
C 5.3023367305 0.2390410668 -1.7300604429
H 5.9590964476 0.6072325758 -2.5120523227
C 5.8025472411 -0.3154188183 -0.5644329763
H 6.8744674063 -0.3645613924 -0.3946126169
N -0.915255535 -1.373137534 -3.1429788382
N 3.3781606451 0.7145619446 -3.1103940499
N 2.5996257968 -1.1742365558 1.0972131917
N -0.8440954655 1.8965465911 0.3297203799
Co 1.1110624435 0.228721224 -1.2008745926
C -1.4706201646 3.1826644176 0.6100051199
H -1.9486671714 3.5340828394 -0.3060260637
H -0.6907431253 3.8968271968 0.8875656111
H -2.2259615163 3.143471726 1.410285554
C 3.0187801909 -2.2495157755 1.9926301128
H 3.4627104723 -3.0474126304 1.3922049874
H 2.1332716976 -2.6451976536 2.4956820653
H 3.7476817884 -1.9431469729 2.7587169416
C 1.4313143247 2.2552768585 -1.462848836
O 0.7731951218 2.8431843102 -2.5406158865
O 2.1196677859 3.0015856282 -0.7675641245
H 4.0780228872 1.0730192938 -3.7478268832
H 1.0271633018 3.7926243853 -2.5311708405

```

Listing S50. Coordinates of 4^(II)-CO₂H, deprotonated.

```

H 2.2579443966 -0.0350055954 3.7495129381
C 1.558424045 0.3424319062 3.0148248683
C 0.5677332615 1.2455259782 3.3747575815
H 0.4649099184 1.5609503447 4.4088553916
C -0.2894596124 1.7507806916 2.4005226002
H -1.0789899215 2.4417118791 2.6655812049
C -0.1374118128 1.3142270361 1.0830283359
N 0.8242542658 0.4326479547 0.7209423245
C 1.6708478088 -0.0331186647 1.6704698085
C -1.7264084853 0.7798711543 -0.6555138752
C -3.1213612542 0.7720061823 -0.6728942009
H -3.6834209068 1.5099583519 -0.1153954922
C -3.7795635842 -0.2291015001 -1.3880196444
H -4.8646609566 -0.2678974506 -1.3995333478
C -3.0379556772 -1.1641652679 -2.0933756468
H -3.5169605446 -1.930136936 -2.6947508746
C -1.6415839282 -1.0739745846 -2.0509492558
N -0.99185326 -0.1480032234 -1.3158197081
N 1.0859595383 -0.666646338 -3.0097033574
C 0.2276016247 -1.5413224586 -3.573044966
C 0.3821357487 -2.020474316 -4.8790461903
H -0.3302861179 -2.7297268697 -5.2878793674
C 1.4358965385 -1.5345368052 -5.6376139716
H 1.5855986067 -1.8830776942 -6.6550334893
C 2.2984896181 -0.586194734 -5.0874400589
H 3.1296622461 -0.1992750409 -5.6624783979
C 2.0982252628 -0.1806088821 -3.767539321
H 5.3728432759 -0.8742997574 1.202685163
C 4.9031395799 -0.542870739 0.2858061113
C 3.5076560789 -0.5141787174 0.1726596999
N 2.8870597181 -0.0929534015 -0.9547141252
C 3.6430536612 0.3441570613 -1.9886129955
C 5.0376859543 0.3694768239 -1.9330372301
H 5.6180927338 0.7073706322 -2.7815455534
C 5.6682830165 -0.0924362727 -0.7807744309
H 6.7523110623 -0.0958326944 -0.7157250204
N -0.8739604823 -1.9456718116 -2.820315612
N 2.9523857427 0.7602183679 -3.14970099
N 2.7001059146 -0.8874531451 1.2555037714
N -1.0057618352 1.7613993288 0.0619051903
Co 0.9470746064 -0.2673579712 -1.0985516026
C -1.6654967187 3.0552488783 0.2626606149
H -2.0865941122 3.3805595213 -0.6908879854
H -0.9135414884 3.783347648 0.5743786139
H -2.4681457712 3.0346860329 1.0131322163
C 3.6354541074 1.7155026808 -4.0274128985
H 2.9028560674 2.1345327675 -4.7204247509
H 4.4588903465 1.2770215201 -4.6083473322
H 4.033502031 2.526297225 -3.4135835082
C 3.2383197747 -1.8496460214 2.2210396085
H 3.7283751085 -2.6527017029 1.6673082476
H 2.4042494262 -2.2820310481 2.7766079399
H 3.9513481508 -1.4064220046 2.9297166374
C 0.9693564032 -2.2599784186 -0.5573043478
O 1.7470953716 -3.1200626258 -0.9490948119
O -0.0023126324 -2.6439963225 0.3660802601
H -1.4118284689 -2.6850862582 -3.2550140368
H 0.1173365592 -3.6064646937 0.5240392696

```

Listing S51. Coordinates of 5^(II)-CO₂H.


```

H 2.2832236789 -0.0232153199 3.7143260416
C 1.5764951712 0.3633157791 2.9906159159
C 0.6099844301 1.2916948283 3.3577653348
H 0.5288472872 1.6185858497 4.3908486777
C -0.2514959717 1.8022653587 2.3919646258
H -1.0279558266 2.506762573 2.660968299
C -0.1351727407 1.3457470611 1.0729920556
N 0.8081843983 0.4437455305 0.7043195767
C 1.6559584602 -0.0258560481 1.6478310154
C -1.7339256714 0.7751280392 -0.6439790606
C -3.1167403693 0.7222692865 -0.5564464136
H -3.6652721225 1.426528195 0.0563380898
C -3.7825574498 -0.3079933726 -1.2501288179
H -4.8635656361 -0.398323351 -1.1764982187
C -3.0598665441 -1.1804543514 -2.0255195184
H -3.5254485302 -1.9644215562 -2.6115397389
C -1.6459521501 -1.0335940928 -2.1484521473
N -0.9994263412 -0.0966556963 -1.3694160046
N 1.0554398216 -0.6066607197 -3.0431006257
C 0.1491771933 -1.4740732398 -3.6161132953
C 0.4385366523 -2.0339294922 -4.8957041781
H -0.2697898436 -2.7538884063 -5.288847453
C 1.533197406 -1.6086162157 -5.6070413496
H 1.7417050913 -2.0117717669 -6.59499957
C 2.3860711534 -0.6332780249 -5.0541142069
H 3.2550409632 -0.2814111053 -5.5956531171
C 2.1091579276 -0.1794356892 -3.7732515102
H 5.3359917397 -0.8826750572 1.2108991239
C 4.8812042503 -0.5409414174 0.2897595626
C 3.4875047272 -0.5183302919 0.1529249227
N 2.8770205097 -0.0870053371 -0.9734691835
C 3.6451621575 0.3664930649 -1.9938210969
C 5.0422275366 0.4046712796 -1.9124080149
H 5.6305267969 0.7539131554 -2.7511966421
C 5.6598610771 -0.0687223998 -0.7591128441
H 6.7434855914 -0.0675461413 -0.6790213138
N -1.0422734472 -1.7816898961 -3.0822147839
N 2.964315799 0.7844879216 -3.1462491683
N 2.6664783489 -0.899770074 1.2241751739
N -1.0025675354 1.784544601 0.064153823
Co 0.9238112259 -0.2384814336 -1.1380923064
C -1.6796792487 3.0614093813 0.2695473456
H -2.1281226004 3.3678831605 -0.6778810669
H -0.9389233345 3.8100521815 0.56433899
H -2.4717431195 3.0341610319 1.0339438517
C 3.6549565148 1.7208034991 -4.0279421681
H 2.9287993396 2.1239715315 -4.737198422
H 4.4845950305 1.2754254307 -4.5986534647
H 4.0508148284 2.5437705055 -3.4263304194
C 3.1704029677 -1.8953649599 2.1652856855
H 3.6341888567 -2.7014711606 1.5926659415
H 2.3210475817 -2.312755443 2.7099689238
H 3.8976676115 -1.4949259183 2.8879711256
C 0.9630670569 -2.2385287714 -0.5730795546
O 1.7655711605 -3.1013401177 -0.9152124636
O -0.0412371869 -2.6369284725 0.3151697916
H 0.0704453268 -3.6052539057 0.4399042454

```

Listing S52. Coordinates of $5^{(II)}$ -CO₂H, deprotonated.

H	2.7267416476	-0.3366588611	3.5660378003	
C	1.9957103303	0.1174469993	2.9098489629	
C	1.0362357349	0.992477937	3.4131587927	
H	1.0012796553	1.2103853477	4.4764849138	
C	0.1196459238	1.5779505022	2.5503661592	O 0.4992845168 2.682526809 -2.6539723808
H	-0.6566312221	2.230998862	2.9275884094	O 1.9848880687 3.0944659205 -1.0303428574
C	0.1874310534	1.2678943241	1.186554768	H 0.6158367462 3.6560576155 -2.7197990903
N	1.1389534907	0.4455370968	0.6858871059	
C	2.0219556671	-0.1275217423	1.5356701905	
C	-1.4187605061	0.8964692792	-0.5844828972	
C	-2.8154304348	0.8963636739	-0.6850120555	
H	-3.4079990551	1.5862959445	-0.0980616816	
C	-3.4240266558	-0.0383322687	-1.5118612545	
H	-4.5059269685	-0.0647642671	-1.6025023356	
C	-2.6410077571	-0.9495958356	-2.2164062108	
H	-3.0985567277	-1.6764130415	-2.8749033536	
C	-1.252581358	-0.8799402744	-2.086037032	
N	-0.6498029911	0.0364182822	-1.2937956283	
N	1.4400600742	-0.3339854536	-3.1042689716	
C	0.5621102478	-1.2036747452	-3.6560954713	
C	0.5938863154	-1.5294032081	-5.013490676	
H	-0.1346216788	-2.209196045	-5.4356874799	
C	1.5581263312	-0.9316112667	-5.8211888131	
H	1.599330167	-1.1608610832	-6.8819225632	
C	2.4730657117	-0.0500432601	-5.261405562	
H	3.2554944338	0.3931700367	-5.863918991	
C	2.3965238657	0.2170009904	-3.8889553301	
H	5.6808789731	-0.8343940088	1.015489162	
C	5.2221290483	-0.4338153775	0.1209072099	
C	3.834758929	-0.4409760959	-0.0332044391	
N	3.2296158858	0.0773664834	-1.126430818	
C	3.9948632424	0.6009601415	-2.1124575677	
C	5.3902042274	0.664732449	-2.0115459164	
H	5.9812730066	1.0809206134	-2.816940144	
C	6.0012126727	0.1400599021	-0.8808288738	
H	7.0821256405	0.171015915	-0.7806253741	
N	-0.406091828	-1.7642949721	-2.7925566808	
N	3.3420515931	1.0461745304	-3.2703473355	
N	2.9899868128	-0.9832843984	0.9625851642	
N	-0.7661731636	1.773587389	0.291715202	
Co	1.2889484728	0.2164470679	-1.2432748492	
C	-1.4168817238	3.0452716055	0.617569908	
H	-1.8419039908	3.458093448	-0.2991171025	
H	-0.6545005184	3.7380073386	0.9789559219	
H	-2.2102682521	2.9505832492	1.3717697097	
C	3.9923104839	2.0828465503	-4.0763387405	
H	3.2379812007	2.5470360503	-4.7140657229	
H	4.808550268	1.7003316965	-4.7045020779	
H	4.3824221731	2.8473659749	-3.4017896137	
C	-0.970399543	-3.0617784211	-3.176890468	
H	-0.1513153341	-3.7270065015	-3.45820253	
H	-1.6826958095	-3.0074723776	-4.0121485042	
H	-1.4794634541	-3.4889753864	-2.3103418951	
C	3.5611652489	-2.0191128796	1.8287093068	
H	4.0754116199	-2.7504024676	1.2015204403	
H	2.7451241179	-2.524517593	2.349609211	
H	4.2705472802	-1.6350231716	2.575228064	
C	1.3243880937	2.2454049773	-1.6157771132	

Listing S53. Coordinates of $6^{(II)}$ -CO₂H.

```

H 2.6252126463 -0.3484213823 3.5256743209
C 2.0215256302 0.2017011547 2.811310072
C 1.2194779253 1.2624246312 3.2157018968
H 1.1726910848 1.544823199 4.2630387769
C 0.4699652066 1.9540085335 2.2672728865
H -0.1908324034 2.7651780059 2.5546292398
C 0.5419350953 1.543196596 0.9382384862
N 1.3519394876 0.5397617821 0.5176795061
C 2.0803293642 -0.1163718443 1.4521120665
C -1.1082990998 1.3465408756 -0.8276207497
C -2.4762119512 1.6030932136 -0.8854338388
H -2.8991281659 2.443037395 -0.3442580987
C -3.2848395965 0.7251959056 -1.6030206956
H -4.3575696209 0.8852006663 -1.6531652346
C -2.7080269244 -0.3628255909 -2.2476296075
H -3.3110452838 -1.0571076313 -2.8236138667
C -1.3213525378 -0.522404065 -2.1866055628
N -0.5212959681 0.3160173817 -1.4857697584
N 1.4465433703 -0.7019729497 -3.2122157314
C 0.4016792848 -1.4126102719 -3.6998401236
C 0.4032166299 -1.9683389726 -4.9816566282
H -0.4571277582 -2.5281866255 -5.3334165659
C 1.4998556924 -1.7449444786 -5.8060352838
H 1.5169416802 -2.1464168226 -6.8146956521
C 2.5798126053 -1.0094373183 -5.3241748126
H 3.4643031707 -0.845833538 -5.9309182779
C 2.5258343785 -0.5331361889 -4.0162418036
H 5.4822920874 -1.8247277803 1.0214952713
C 5.1354166069 -1.4083818837 0.0814493223
C 3.8041523765 -1.0086523244 -0.0594206084
N 3.3194524622 -0.479819423 -1.2083245031
C 4.1769662338 -0.3385303968 -2.249735593
C 5.5291933602 -0.6629859694 -2.1687932881
H 6.1771610401 -0.5289708111 -3.0286556433
C 6.0082074645 -1.2134718585 -0.9826156802
H 7.0530546752 -1.4943985515 -0.8918186389
N -0.7160485195 -1.5750888476 -2.8775243309
H -1.3895426349 -2.2305449859 -3.2585157354
N 3.6279124531 0.1315404338 -3.4539235396
H 4.337500053 0.3607312628 -4.14248049
N 2.9254295262 -1.1408821871 1.0185736255
N -0.2653107389 2.147430679 -0.0395569712
H -0.7294591444 2.98347643 0.3009170108
Co 1.438131592 0.0858949284 -1.4019687764
H 3.3257832787 -1.668281395 1.7866295919
C 1.887292369 2.0298533493 -2.0387555997
O 2.1281915166 3.0838976707 -2.3791503838

```

Listing S54. Coordinates of $\mathbf{1^{(II)}}\text{-CO}$.

```

H 2.5445345817 -0.3424374231 3.5337784534
C 1.9423457026 0.2208668442 2.8311500532
C 1.0490381154 1.1817742171 3.2312131709
H 0.8978076994 1.3929648945 4.285830115
C 0.3188466455 1.8935880175 2.2578413387
H -0.4177636336 2.6407638419 2.5345031339
C 0.5223410513 1.5664856619 0.9326813592
N 1.4159297731 0.6380730344 0.5023949712
C 2.1893874575 -0.0169356205 1.444562781
C -1.0960658229 1.3865747423 -0.8436368585
C -2.4710403733 1.6254357445 -0.9256899039
H -2.905986298 2.4758556281 -0.411313457
C -3.2611817882 0.7149773159 -1.6166025127
H -4.3358128948 0.8575613402 -1.6789476974
C -2.6653007351 -0.3899529899 -2.2173652385
H -3.2530212237 -1.1140864099 -2.7718661007
C -1.2772178481 -0.5258656012 -2.1385758952
N -0.4927314086 0.3460695832 -1.4686881139
N 1.4756020324 -0.674259047 -3.1961866444
C 0.4403152391 -1.4161673538 -3.6461877422
C 0.4144492775 -1.9858780996 -4.9214078483
H -0.4425571827 -2.5700479252 -5.2399483418
C 1.4817229802 -1.7429320181 -5.7808544513
H 1.4794699836 -2.1557038483 -6.7851823035
C 2.5550452378 -0.9797089327 -5.3380098139
H 3.4214858006 -0.8039445691 -5.9667704355
C 2.5312542551 -0.4937422009 -4.0273892577
H 5.497418942 -1.8537653679 0.9510629291
C 5.1657993314 -1.4343547476 0.0088736229
C 3.8525813859 -0.8731029674 -0.0129496545
N 3.3580680501 -0.3664568026 -1.2020669284
C 4.1839749357 -0.3264254138 -2.2800719344
C 5.4897658671 -0.7731286652 -2.2757713352
H 6.0940074525 -0.7187804555 -3.1753594401
C 5.9822844136 -1.3557577477 -1.0904763421
H 6.9970141116 -1.7415153174 -1.0556887562
N -0.6520098373 -1.5953606718 -2.7897760885
H -1.318653544 -2.2668556742 -3.1523534909
N 3.6222414008 0.1825469066 -3.4875925064
H 4.3390995452 0.373742051 -4.1793797386
N 3.2148179143 -0.8239664431 1.1597203588
N -0.2659866735 2.1977648857 -0.0740815929
H -0.7508757125 3.0111275989 0.2896668172
Co 1.4994171118 0.1888188804 -1.3927467857
C 1.9307689481 2.0701033645 -2.0117009461
O 2.3148797332 3.1245777607 -2.1981309482

```

Listing S55. Coordinates of $\mathbf{I}^{(III)}$ -CO, deprotonated.

```

H 2.6591338127 -0.3457988678 3.5039014168
C 2.0620120701 0.1966665961 2.7828074822
C 1.3162842813 1.3051229112 3.1778079817
H 1.3222441329 1.6233201551 4.2159699878
C 0.5543967186 1.9905124025 2.2394302552
H -0.0726645677 2.8293075712 2.5235287545
C 0.5711371788 1.5359620305 0.9209166738
N 1.3404333096 0.5022787678 0.5081492002
C 2.0665980204 -0.175180249 1.4366683679
C -1.1101907201 1.3316027181 -0.8250075497
C -2.4773035831 1.5953934942 -0.8746558209
H -2.8942019335 2.4333549225 -0.3258098328
C -3.2930149515 0.7278634075 -1.5970664453
H -4.3650266468 0.8942251282 -1.6414169623
C -2.7252335331 -0.3563202951 -2.2564694783
H -3.334668174 -1.0399022211 -2.8385010638
C -1.3393923124 -0.5251777449 -2.2009837728
N -0.5341098671 0.3008838794 -1.491967805
N 1.4318104777 -0.7166694061 -3.2170746417
C 0.3870227001 -1.4193737437 -3.7153176927
C 0.3997428905 -1.975115818 -4.9972265098
H -0.4597376938 -2.5296416882 -5.3594513695
C 1.5078429933 -1.7586556932 -5.8082341109
H 1.5346007083 -2.1615548707 -6.8161092182
C 2.585545189 -1.026196388 -5.3162484087
H 3.4760709959 -0.8653030531 -5.914809544
C 2.5192308814 -0.5472345588 -4.0096798397
H 5.4665932763 -1.7932073419 1.0419526907
C 5.1099359287 -1.3754712115 0.1097003719
C 3.7612489211 -1.0500716982 -0.0501034523
N 3.2915818346 -0.5066501043 -1.2044146951
C 4.1578741261 -0.3175525348 -2.226483656
C 5.5245228679 -0.5753457392 -2.1205063935
H 6.1838064022 -0.400706332 -2.9645079256
C 5.999280791 -1.1108143504 -0.929437331
H 7.0555639694 -1.3333919858 -0.8119263542
N -0.7411905323 -1.5732078472 -2.9054790017
H -1.4188482476 -2.2178933591 -3.2971374287
N 3.6122782036 0.1270616627 -3.4412996039
H 4.3228869908 0.366129491 -4.125223559
N 2.8317167258 -1.2663089571 0.9842882612
N -0.2579780199 2.1294842389 -0.0442801171
H -0.7122983075 2.9713078913 0.2945278936
Co 1.4173532075 0.0514952344 -1.4041467893
C 3.148058931 -2.3208677845 1.9646129707
C 1.875431478 2.0034300845 -2.0341819732
O 2.1214834295 3.0575091166 -2.3713157791
H 3.4765384807 -3.2087362149 1.4217793027
H 2.2359968773 -2.5703120882 2.5094407616
H 3.9260702879 -2.0315295569 2.6817617534

```

Listing S56. Coordinates of 2^(H)-CO.

```

H 2.6305003732 -0.4008221661 3.4594440185
C 2.048632942 0.1726685956 2.7500439866
C 1.3355854331 1.2974256123 3.1645985341
H 1.3506508652 1.5962207565 4.2085490146
C 0.5933806127 2.0177161092 2.240962691
H -0.013519358 2.8668371614 2.5375571941
C 0.5887665171 1.5813506292 0.9111394256
N 1.3344749633 0.5381324885 0.4811931192
C 2.0373901601 -0.1725988782 1.397199493
C -1.1020403957 1.3591470098 -0.8022362095
C -2.4657998254 1.5557087917 -0.7175248715
H -2.8721675593 2.3433278423 -0.0914860003
C -3.3030980036 0.663872761 -1.4179164533
H -4.3822054727 0.7706386923 -1.3555428501
C -2.7423658597 -0.3369207497 -2.1709112218
H -3.3383918607 -1.0355313996 -2.7456984776
C -1.3246805271 -0.4444832965 -2.3041226291
N -0.5167316041 0.3917099147 -1.5544198655
N 1.4227234044 -0.6143311264 -3.2573145659
C 0.3370769452 -1.3084129028 -3.7611301933
C 0.4804266275 -2.0141469333 -4.9943045583
H -0.3806977696 -2.576574683 -5.3346449337
C 1.6272956097 -1.9012973003 -5.7391445128
H 1.7154226578 -2.4031461525 -6.6983785027
C 2.6991760013 -1.1289282565 -5.2475338905
H 3.6309859712 -1.0366071617 -5.7957590669
C 2.5512280739 -0.5373765625 -4.009118251
H 5.4050306141 -1.8155342488 1.0320722934
C 5.0730924419 -1.3752515705 0.1011275547
C 3.7304815249 -1.0419181658 -0.0871779534
N 3.2871772473 -0.4703473373 -1.233842162
C 4.1728494108 -0.2682479996 -2.2358967459
C 5.5415750004 -0.5273461008 -2.0995019204
H 6.216797439 -0.3386495497 -2.9276270779
C 5.987501203 -1.0877950752 -0.9121934966
H 7.0401318826 -1.3173163112 -0.77565595
N -0.8799779686 -1.3218763464 -3.2090710919
N 3.6420423259 0.1834032166 -3.4408001005
H 4.3581779878 0.3843668523 -4.1303273165
N 2.7747621813 -1.2758037668 0.9222358723
N -0.2247378044 2.1870474182 -0.042497747
H -0.702006541 3.0063035281 0.3176158723
Co 1.4118335287 0.1486248591 -1.4678472049
C 3.0548383814 -2.3577220997 1.8745559323
C 1.8436266192 2.0364332879 -2.0908227234
O 1.9275741153 3.0522767233 -2.596307852
H 3.3734466267 -3.2379012163 1.3128180607
H 2.1301704678 -2.602186889 2.4009245695
H 3.8289043941 -2.1075380041 2.6126187642

```

Listing S57. Coordinates of $2^{(II)}$ -CO, deprotonated.

```

H 2.670253747 -0.325271233 3.5291932737
C 2.0683243266 0.2034887047 2.8019542351
C 1.3070577183 1.3053672092 3.1862343205
H 1.3049034017 1.6300399532 4.2224025447
C 0.5430593484 1.9781541897 2.2403604237
H -0.0916529749 2.8137657896 2.5166558927
C 0.5710934145 1.5166158179 0.9242825808
N 1.3483224537 0.4839527853 0.5246640273
C 2.0807400789 -0.1784948869 1.4586469866
C -1.0889146668 1.319673706 -0.8525026133
C -2.4461013579 1.6238582974 -0.959628591
H -2.8584633723 2.4864232172 -0.4463844226
C -3.253416639 0.7643346255 -1.6947490156
H -4.3162068152 0.9634196586 -1.7943404318
C -2.6954157722 -0.3622764738 -2.2953846259
H -3.3135721163 -1.0358867759 -2.8741016552
C -1.3211718158 -0.5830604159 -2.1805957946
N -0.5222674518 0.261251288 -1.4759883328
N 1.4264767065 -0.7462988297 -3.1857476144
C 0.3763019627 -1.4607292553 -3.6698716058
C 0.3641652568 -1.9441853031 -4.9800748584
H -0.4875408792 -2.4969498772 -5.3539661713
C 1.4431055512 -1.6640084241 -5.8159755243
H 1.4387818426 -2.0120965835 -6.8445111749
C 2.5276671167 -0.9480721056 -5.3239112459
H 3.3999718374 -0.7501288089 -5.938203382
C 2.4906486481 -0.5315114661 -3.9931058038
H 5.4980121803 -1.7865553533 1.0485384232
C 5.1293333989 -1.3780494471 0.1168722643
C 3.7783951283 -1.0559330946 -0.0308570841
N 3.2967587749 -0.5237521734 -1.185166323
C 4.1513640958 -0.3341070015 -2.2167160225
C 5.5189863204 -0.5927708601 -2.1242279559
H 6.1699379582 -0.4213867682 -2.9753003326
C 6.0060849129 -1.1220399969 -0.9352824336
H 7.0635547363 -1.3442373001 -0.8282061076
N -0.7048245362 -1.6885877647 -2.7971817024
C -1.5482154382 -2.8680540156 -3.0637311346
N 3.5961073289 0.1204381199 -3.4235103198
H 4.3003635987 0.3707117774 -4.1098359286
N 2.8593007948 -1.2644440823 1.0151048734
N -0.2467436746 2.1079940953 -0.0518995501
H -0.6979088796 2.9558952333 0.2754627915
Co 1.4199106413 0.0089096639 -1.3764330238
C 3.1920416861 -2.304099916 2.0059402205
C 1.8735774512 1.9774747745 -2.0207018161
O 2.1155026586 3.0308203588 -2.3633804364
H 3.5260809465 -3.1952705909 1.4718859335
H 2.2859533496 -2.556379461 2.5594515002
H 3.9715314469 -1.9980440702 2.7145565398
H -0.8964555441 -3.7223256268 -3.2547458172
H -2.2255872672 -2.7365275913 -3.9165277561
H -2.1372616182 -3.0803637125 -2.1698902238

```

Listing S58. Coordinates of 3^(II)-CO.

```

H 2.9068788053 -0.2211540924 3.4700172567
C 2.2309856941 0.2639484683 2.7778123323
C 1.4975059212 1.4036150032 3.1663476169
H 1.6060843816 1.7958169743 4.1735668788
C 0.6427781595 2.0014678642 2.273582783
H 0.02820412 2.8548096568 2.5347177962
C 0.4702676626 1.4514097164 0.9711146302
N 1.2740371576 0.4014968337 0.5740551265
C 2.0995479318 -0.1877556146 1.4772439652
C -1.1357016066 1.2607248471 -0.7477994784
C -2.4741621987 1.631596516 -1.0634324395
H -2.8721958422 2.5109550937 -0.5710913034
C -3.2301403694 0.842165034 -1.8943685322
H -4.2634630189 1.0988990211 -2.109858879
C -2.6657807701 -0.3182566134 -2.4625458312
H -3.2486982835 -0.9532507218 -3.1170187897
C -1.3368281584 -0.5966315879 -2.1994544674
N -0.5673965889 0.1824760623 -1.3961515925
N 1.3892428856 -0.7358656121 -3.1573667356
C 0.3737449184 -1.4976601849 -3.6463831601
C 0.4100517351 -2.0085834878 -4.9511343559
H -0.4128577993 -2.6009325912 -5.3284911639
C 1.4860206903 -1.6913774395 -5.7730204701
H 1.5141104244 -2.0541697596 -6.7962588722
C 2.5284643936 -0.9149906841 -5.2772789657
H 3.4013163368 -0.6853948747 -5.879541437
C 2.4499077087 -0.4847957725 -3.9524893555
H 5.489556264 -1.9007719996 0.9851529845
C 5.1107913251 -1.4505965063 0.0771645588
C 3.7587405202 -1.0949501374 -0.0250705652
N 3.2642809378 -0.5127615321 -1.1508463314
C 4.1025203426 -0.2889668085 -2.1842590778
C 5.4685102647 -0.5673479039 -2.1322024004
H 6.1038030413 -0.3669383814 -2.9886502791
C 5.9691164966 -1.160300596 -0.9776363369
H 7.0252061138 -1.4017972219 -0.9016092841
N -0.7007252376 -1.733973671 -2.7889874097
C -1.5523470044 -2.8935460322 -3.0741069596
N 3.5265031048 0.2087542367 -3.3682777752
H 4.2258481162 0.4771048937 -4.0518180953
N 2.8568400012 -1.3102567161 1.0166440423
N -0.517973801 1.960575844 0.2177634965
Co 1.3531475169 -0.0262790823 -1.3102008489
C 3.2051487495 -2.3270273032 2.0145240536
C 1.715242142 1.9646946277 -1.8705935464
O 1.9161050186 3.0399151717 -2.1769522037
H 3.5116370195 -3.2384346611 1.4957621864
H 2.313007588 -2.5463773571 2.6034792564
H 4.0094468401 -2.0191400779 2.6968190187
H -0.9156032536 -3.7665340744 -3.2359924119
H -2.2015034389 -2.7600640108 -3.9503846973
H -2.179382958 -3.0787727553 -2.2004139304

```

Listing S59. Coordinates of $3^{(II)}$ -CO, deprotonated.


```

H 2.5716784129 -0.4017656552 3.4957675504
C 2.0011455252 0.1629276724 2.770335327
C 1.2562444606 1.2686038734 3.1653163531
H 1.2293467635 1.561173304 4.2107584058
C 0.5365862996 1.9921941161 2.2195786391
H -0.0779113454 2.8313221301 2.5180407297
C 0.5817153793 1.5769652659 0.8881985097
N 1.3458438459 0.528699662 0.485396108
C 2.0390767324 -0.1765597673 1.4151646516
C -1.0777890419 1.3678381606 -0.8306644939
C -2.4537121148 1.5885961116 -0.841660152
H -2.8835610784 2.4234915233 -0.3037853511
C -3.2734475748 0.6829163313 -1.5150332596
H -4.3503773047 0.8215816811 -1.5186052872
C -2.7060638945 -0.3958827728 -2.1782732263
H -3.3177809416 -1.1029888444 -2.7291475075
C -1.3142501882 -0.5288850064 -2.1661726614
N -0.5093693692 0.3241680764 -1.4941682159
N 1.4478304713 -0.7056555888 -3.2226108738
C 0.3992915549 -1.4106353633 -3.7082913095
C 0.4008308509 -1.9677247237 -4.9896115689
H -0.4617565695 -2.5219531953 -5.3447614754
C 1.5043807152 -1.7552723011 -5.8083889447
H 1.5228651589 -2.1599440464 -6.8157425639
C 2.5893532729 -1.0275760559 -5.3250562486
H 3.477249118 -0.8739323102 -5.9294130068
C 2.5330005716 -0.5444394219 -4.0193920198
H 5.4524208516 -1.7803086583 1.0496098744
C 5.1039288081 -1.3634368305 0.1138013292
C 3.7570643767 -1.0380291203 -0.0589960419
N 3.300905622 -0.4929340596 -1.2170239641
C 4.1724021257 -0.3129313995 -2.2355246497
C 5.5376820403 -0.5741122809 -2.1181635276
H 6.2040182974 -0.4071228196 -2.9581743409
C 6.0016940823 -1.103113025 -0.919775149
H 7.0567121633 -1.3265525958 -0.7928463136
N -0.7166809367 -1.5700012446 -2.8825273828
H -1.3937236167 -2.2231787439 -3.2608575406
N 3.632995508 0.1234160142 -3.4562697855
H 4.3459854433 0.3515683794 -4.1413742047
N 2.8126216114 -1.2619438395 0.9608248848
N -0.198969972 2.2045333073 -0.106974398
C -0.6359873851 3.5892807582 0.1425701851
Co 1.4352281567 0.0773280617 -1.4199540722
C 3.1142168646 -2.330138037 1.9309267175
C 1.8917447278 2.0137943668 -2.0511154602
O 2.134166915 3.0703951064 -2.3868098228
H -1.004354387 4.0095500139 -0.7949030771
H 0.2288892459 4.1723738735 0.4641653075
H -1.422695145 3.6676418287 0.902862071
H 3.4538090776 -3.2094066834 1.3809548216
H 2.193659637 -2.5900587142 2.4563651621
H 3.8793761778 -2.0498665135 2.6653012692

```

Listing S60. Coordinates of 4^(II)-CO.

```

H 2.5864405033 -0.3786950557 3.4446083685
C 2.0248630119 0.2054485773 2.7274892597
C 1.3436658165 1.3530811136 3.124565007
H 1.3593165429 1.6609978613 4.1660107718
C 0.6285968441 2.0914633602 2.1907462578
H 0.053476204 2.9573077787 2.4914426362
C 0.6080267426 1.6481739172 0.8624521239
N 1.3322093165 0.5736287051 0.4543197533
C 2.0098022036 -0.1481239989 1.3760085044
C -1.0777218857 1.3559157726 -0.8000906078
C -2.4442703105 1.4673745842 -0.6407251239
H -2.8709183296 2.240610983 -0.0148236275
C -3.267415867 0.5130235969 -1.2765907479
H -4.3449155156 0.5574226566 -1.1460266896
C -2.6989996564 -0.4593375403 -2.0578502938
H -3.2868377164 -1.1955040695 -2.5931851947
C -1.2869219256 -0.4848127731 -2.2728786886
N -0.490285396 0.3964651941 -1.5667146856
N 1.451864036 -0.598201304 -3.2726748663
C 0.3611764712 -1.2745204136 -3.7882127086
C 0.486374835 -1.9246003202 -5.0528516441
H -0.3812755403 -2.4673041278 -5.4082205114
C 1.6291870551 -1.7913900528 -5.8014580297
H 1.7050110144 -2.2533528559 -6.7815733609
C 2.7146285893 -1.0563583296 -5.2845697913
H 3.6462730901 -0.9587449531 -5.8322449978
C 2.5799336334 -0.5101177072 -4.0234483234
H 5.3457435242 -1.8842418595 1.0528571961
C 5.0349266649 -1.4330380777 0.1198546768
C 3.7038156742 -1.0629139087 -0.0818480441
N 3.2903661947 -0.4773563257 -1.2321499578
C 4.1894408179 -0.2968363816 -2.2253461329
C 5.5490590425 -0.594103871 -2.0754968087
H 6.2382799067 -0.4232963788 -2.8959488416
C 5.9665433929 -1.1686806798 -0.8842352906
H 7.011047068 -1.4273316094 -0.7376000628
N -0.8430409093 -1.329349617 -3.2087648145
N 3.6828799179 0.1730095893 -3.4342858799
H 4.4114763825 0.3630170756 -4.1136879244
N 2.7274432361 -1.2719676522 0.9126330531
N -0.186142808 2.2491504323 -0.1168653728
C -0.6664067723 3.6124196063 0.1280130904
Co 1.4299478618 0.1655618366 -1.4848946305
C 2.968461237 -2.3567593817 1.8720694237
C 1.8701737184 2.0410196889 -2.106982873
O 1.9412171198 3.0639577934 -2.6027465357
H -1.0995045559 3.9931760346 -0.7984560889
H 0.184708263 4.2421317508 0.3986910199
H -1.4230074345 3.6766585682 0.9218305987
H 3.2697710385 -3.2476533669 1.3175705892
H 2.0320504887 -2.5748739889 2.3891572171
H 3.7407371636 -2.124359876 2.6178896035

```

Listing S61. Coordinates of 4^(II)-CO, deprotonated.

H 2.5686918436 -0.3955003506 3.5215910875
 C 1.9951507287 0.1578642637 2.7898499493
 C 1.2303891123 1.2531544822 3.1758488126
 H 1.1895560216 1.5463370403 4.2206648774
 C 0.5117261068 1.9679391031 2.2224127931
 H -0.1139061824 2.8013649267 2.5138233065
 C 0.576219961 1.5533700854 0.891639743
 N 1.3506416977 0.5086354931 0.5006245457
 C 2.0478056178 -0.1851309319 1.4357159408
 C -1.0597130243 1.3619020869 -0.8613228502
 C -2.4282701416 1.6254781321 -0.9319432903
 H -2.8543650342 2.4846980815 -0.4307562049
 C -3.2420504068 0.7296332061 -1.6186473049
 H -4.3122818933 0.903304836 -1.6795924512
 C -2.6839067483 -0.392784487 -2.2206223504
 H -3.3061260751 -1.0876104857 -2.7689882589
 C -1.3008437451 -0.5809730609 -2.146449645
 N -0.5013414531 0.2893932189 -1.4795066144
 N 1.4391328794 -0.7310292463 -3.1928877558
 C 0.3845581177 -1.4469356918 -3.6629856649
 C 0.3595511723 -1.9324104454 -4.9722601743
 H -0.4963074163 -2.4844617555 -5.3378504613
 C 1.4334621379 -1.6576102535 -5.8168995193
 H 1.4196318997 -2.0078009786 -6.844644827
 C 2.5264866391 -0.9472825688 -5.334990262
 H 3.3957761236 -0.7575674252 -5.9561238732
 C 2.5009329098 -0.5259837837 -4.0052105212
 H 5.4829391602 -1.7686578692 1.0539830994
 C 5.12201687 -1.3615648316 0.1185806541
 C 3.7720122827 -1.0420523082 -0.0423042011
 N 3.3032668427 -0.508560451 -1.2004057613
 C 4.1631321189 -0.3265270289 -2.2283692246
 C 5.530047898 -0.5856064327 -2.1239292962
 H 6.188073375 -0.4201761942 -2.9707452095
 C 6.0070947389 -1.1077412139 -0.9275683284
 H 7.0638377632 -1.3284910193 -0.8107158376
 N -0.6826839579 -1.6796208429 -2.7743873494
 C -1.5138193016 -2.8717630739 -3.0222736587
 N 3.6141003163 0.1180993105 -3.4416350282
 H 4.3205056849 0.3577848684 -4.1294184422
 N 2.8391516493 -1.2610622027 0.9895515435
 N -0.1873869951 2.1849202238 -0.115116771
 C -0.6065730991 3.5771562649 0.1242183996
 Co 1.4352668498 0.0392341855 -1.3943798321
 C 3.1586156524 -2.3162838812 1.9682887411
 C 1.8886614663 1.9869604208 -2.0363551344
 O 2.1259264436 3.0439970008 -2.3750330491
 H 3.5075868078 -3.1961677076 1.4253007111
 H 2.2439870128 -2.5832096802 2.5004683478
 H 3.9232526355 -2.0184288707 2.6962946403
 H -0.9420317393 4.0052794405 -0.8220604106
 H 0.259289243 4.1446523444 0.4697768297
 H -1.4118708476 3.6678705405 0.8633426149
 H -0.8535819822 -3.7162073025 -3.2270182992
 H -2.2108726738 -2.7508898024 -3.8606940212
 H -2.0806550633 -3.0928573781 -2.116264753

Listing S62. Coordinates of 5^(m)-CO.

```

H 2.4639876532 -0.4592769256 3.5527002179
C 1.9252945066 0.106243269 2.8040731766
C 1.1710421974 1.2147914657 3.1633724774
H 1.0979152949 1.5074353765 4.2067879888
C 0.5049871862 1.9496287226 2.1851741067
H -0.1140004404 2.7958769368 2.4528825761
C 0.6101570506 1.53099585 0.8582831821
N 1.3732592929 0.474446747 0.490758206
C 2.0300341596 -0.2325241699 1.4467732356
C -1.0200279327 1.342250015 -0.8903083368
C -2.3876546904 1.6176466356 -0.9236758888
H -2.7901867637 2.4924279548 -0.4299807229
C -3.2284653703 0.70691571 -1.5592661837
H -4.2992588189 0.88615702 -1.5903975109
C -2.6973136006 -0.4317000909 -2.1495233352
H -3.338247923 -1.1353428725 -2.663880733
C -1.3080659885 -0.6241471767 -2.1244122095
N -0.4854599476 0.2557806599 -1.496812783
N 1.4575746512 -0.8393137601 -3.1708963361
C 0.3562199341 -1.4544563584 -3.67185373
C 0.241050162 -1.8118126782 -5.0032444005
H -0.6550257676 -2.2909275492 -5.3760667228
C 1.3048134687 -1.495660603 -5.8729199416
H 1.2264050072 -1.7392768077 -6.928710003
C 2.4373632776 -0.8960397682 -5.3786480546
H 3.2971335721 -0.6713436477 -5.9986706876
C 2.5507885002 -0.6240197257 -3.9854385146
H 5.4907732067 -1.5422881106 1.1913928415
C 5.132382931 -1.2159473963 0.2236343324
C 3.7808270524 -1.0421793079 -0.0136824848
N 3.2950914191 -0.6196524255 -1.2085206957
C 4.1575157441 -0.4283412792 -2.2687860774
C 5.5607632572 -0.5109844383 -2.0399346717
H 6.2126322055 -0.3080750175 -2.8813930237
C 6.0359629297 -0.914143425 -0.8159442445
H 7.1041955647 -1.013866113 -0.6452915388
N -0.7055703435 -1.7159118602 -2.7505103512
C -1.5426770986 -2.8884697628 -3.0251505026
N 3.7498780204 -0.2214107609 -3.5320713973
N 2.819349359 -1.2980063982 1.0135900386
N -0.1207256388 2.16643977 -0.1734385652
C -0.5054368104 3.5672880432 0.0343769874
Co 1.4612610812 -0.0504429893 -1.4086133677
C 3.163280801 -2.3325285294 1.9947267644
C 1.9849495901 1.8402090333 -2.1107571807
O 2.2542464096 2.8818717086 -2.4787578473
H 3.5592832578 -3.1947780499 1.4557716376
H 2.2544520672 -2.6382535733 2.5184962095
H 3.9082870023 -2.0088802239 2.7346052204
H -0.8283799873 3.9832048659 -0.9221108361
H 0.3733300312 4.121086787 0.3707225844
H -1.3109936849 3.6996127023 0.7691067253
H -0.8870938683 -3.7231073511 -3.2789084121
H -2.2552681784 -2.7390075255 -3.8480187715
H -2.0972349911 -3.1459026016 -2.1196224457

```

Listing S63. Coordinates of 5^(m)-CO, deprotonated.

```

H 2.5817151623 -0.3981234165 3.5006608926
C 2.0046447664 0.1613663779 2.7762618121
C 1.2447851315 1.2564101988 3.1738762338
H 1.2133555757 1.5442596807 4.2204998241
C 0.5161803736 1.9759103376 2.231412206
H -0.1088851275 2.8057670492 2.5340513525
C 0.5702951149 1.5696948672 0.8972605844
N 1.3452426747 0.5299498189 0.495785457
C 2.0440649534 -0.1749938852 1.4201840795
C -1.066550322 1.3799994114 -0.8578812911
C -2.4362810729 1.6359665603 -0.9396933533
H -2.8724967459 2.4906397976 -0.4394244114
C -3.2383591101 0.7372699274 -1.6366161758
H -4.3087194086 0.9062024714 -1.70780357
C -2.6700974018 -0.3837190569 -2.2327095057
H -3.284467855 -1.082987475 -2.784457605
C -1.2872557287 -0.5658799698 -2.1442368696
N -0.4991944323 0.3129907554 -1.4763607867
N 1.4510671038 -0.6975447412 -3.1881698521
C 0.4160552688 -1.4510368545 -3.6362580705
C 0.4095665451 -1.9866472269 -4.927255174
H -0.4310582233 -2.5705079756 -5.2782419297
C 1.4832047479 -1.7188320432 -5.769994045
H 1.4902128303 -2.1120949493 -6.7822105938
C 2.5532346844 -0.9561001117 -5.3116932167
H 3.4114501351 -0.7736319689 -5.9450686172
C 2.5160121731 -0.4779602458 -4.0009524191
H 5.4405093174 -1.8617932364 0.9971447098
C 5.0888225466 -1.4209057683 0.0737112615
C 3.7489991651 -1.0518109795 -0.0748999826
N 3.2959013944 -0.4773350126 -1.2169441411
C 4.1551492685 -0.2789194254 -2.2491374072
C 5.5113809158 -0.5930115524 -2.1491792907
H 6.1819389163 -0.4292061232 -2.9825446565
C 5.9731819379 -1.1707293219 -0.9703514766
H 7.0217104449 -1.4344520251 -0.8687509036
N -0.6572918837 -1.6704434877 -2.7508133808
C -1.4791207563 -2.8733095422 -2.9755566997
N 3.6010939815 0.2339056836 -3.4428239752
C 4.5118528716 0.9224402587 -4.373967406
N 2.8166323289 -1.2595341396 0.9605887622
N -0.2042081416 2.2028840923 -0.1000978263
C -0.6362763042 3.5883423734 0.1533386723
Co 1.4358551321 0.0790080475 -1.3993692797
C 3.116322302 -2.3296229326 1.9290647853
C 1.8817812906 2.0121769269 -2.0321832508
O 2.1240815569 3.0680119643 -2.3748349061
H 3.4396915579 -3.214339569 1.378025469
H 2.1989806945 -2.5779112781 2.465535355
H 3.8926061854 -2.0559917475 2.65426834
H -0.976145674 4.0232600889 -0.7882261299
H 0.2240606151 4.1608704619 0.5042812945
H -1.4421169302 3.6632707393 0.8937258931
H -0.8129096178 -3.7195902594 -3.1516396693
H -2.1687978228 -2.7783437577 -3.8233852239
H -2.0537346071 -3.0740162016 -2.0697505213
H 3.9126192282 1.4833855191 -5.0932574147
H 5.1757572744 0.2388058226 -4.9171475647
H 5.1177309987 1.6309470482 -3.8063183911

```

Listing S64. Coordinates of 6^(II)-CO.

```

H 2.1851711818 -0.5571487609 3.7325851033
C 1.5371712452 -0.0212590044 3.0438088873
C 0.4018651552 0.6363571665 3.4918974006
H 0.1370303279 0.6178511194 4.5455374975
C -0.3764009463 1.3404019589 2.5701038341
H -1.2578465342 1.8996896144 2.8604680387
C 0.0008699854 1.3312711748 1.2313642333
N 1.0950479081 0.6674045094 0.7666008833
C 1.8621186346 0.0409566535 1.6759986325
C -1.5529773355 1.0705948193 -0.4905356273
C -2.914308844 0.922544273 -0.2469425828
H -3.3838683977 1.5577700529 0.4947143377
C -3.6269533164 -0.0329525522 -0.9751254401
H -4.6910261683 -0.1792339425 -0.8109286382
C -2.9570835477 -0.7791304872 -1.9325014084
H -3.4796029702 -1.5138853401 -2.5396410528
C -1.5834753144 -0.5491231451 -2.1340113088
N -0.871237883 0.3295374118 -1.4070769066
N 1.3167034738 -0.5916497543 -3.2360914994
C 0.1971938061 -1.0012189549 -3.8770428109
C 0.1241606503 -1.2227780408 -5.2565168282
H -0.8157456203 -1.5164745735 -5.7138489224
C 1.2691973199 -1.0215535869 -6.0245471512
H 1.2442134038 -1.1623236934 -7.1012839122
C 2.4393162976 -0.6466264256 -5.3909701557
H 3.3607108645 -0.5057847193 -5.9480920292
C 2.4299670568 -0.4715859821 -3.9917224573
H 5.6166039721 -0.3652509284 1.3937246648
C 5.2270423822 -0.3086637119 0.3818929282
C 3.8473567552 -0.3551647471 0.1548022558
N 3.2795043041 -0.2461230751 -1.0688036417
C 4.1260737243 -0.1660293423 -2.1180394663
C 5.5270193733 -0.0835392942 -1.9783520784
H 6.1545305558 0.0114687322 -2.8594973811
C 6.0763602442 -0.1510044196 -0.7115393543
H 7.1516324445 -0.0880326103 -0.5714072514
N -0.9514065808 -1.294108426 -3.1301681842
H -1.6144929408 -1.8343772518 -3.6699553418
N 3.6565328685 -0.217239357 -3.4139082234
H 4.3693590326 0.0034791097 -4.0948887242
N 3.0328262858 -0.599145909 1.2682600062
N -0.8012411577 2.0052393496 0.2713777191
H -0.1672463408 2.5315843886 -0.3809001057
Co 1.2556860123 0.3472828104 -1.3324821686
H 3.573823076 -0.9279026861 2.0570443283
C 1.6504375798 2.2397011083 -1.9878610484
O 2.5588188322 2.2793912283 -2.8278189904
O 0.9399791439 3.1365952411 -1.4736400589

```

Listing S65. Coordinates of **1^(f)-CO₂** forming one intramolecular hydrogen bond. (Corresponds to the structure labeled “1 H-bond” in Figure S49.)

```

H 2.997971616 0.9369953733 3.4137810464
C 2.1222517727 1.1081690786 2.7949361938
C 1.2353734267 2.1559805476 3.0645458967
H 1.403469991 2.8105086421 3.915412704
C 0.1269880035 2.3317078255 2.2528754761
H -0.6208096872 3.0897742005 2.4615835859
C -0.0555453015 1.455856072 1.1672550035
N 0.8450355328 0.5097897868 0.8381044045
C 1.8788512894 0.3146194552 1.6748220464
C -1.7322742691 0.5030619726 -0.4015793364
C -3.057637043 0.1289875517 -0.203664852
H -3.6058403481 0.5660319699 0.6231752478
C -3.6423331262 -0.7977519786 -1.0713849683
H -4.6725148165 -1.1154997157 -0.9405139035
C -2.8767409894 -1.2837486359 -2.1203591705
H -3.2942174747 -1.9738014847 -2.8492530304
C -1.547225633 -0.8493111658 -2.2542458457
N -0.9357601069 -0.0239705794 -1.3758626042
N 1.3395182892 -0.4165863082 -3.251532404
C 0.2625325332 -0.7149991912 -4.0095979169
C 0.224095116 -0.5506024238 -5.3982757014
H -0.6861534681 -0.7611521719 -5.9511802024
C 1.3666996145 -0.0699360764 -6.0383759285
H 1.3654754705 0.0980335187 -7.1116387392
C 2.5066975834 0.1779515924 -5.2923006365
H 3.4254454618 0.52073765 -5.7587593173
C 2.4609251688 -0.0519711806 -3.9026835913
H 5.21617616 -1.588367293 1.4842092808
C 4.905046803 -1.2728765089 0.4926320958
C 3.5969784417 -0.8144141662 0.2785091018
N 3.1252297337 -0.4156645991 -0.9234566708
C 4.0176437029 -0.3992863989 -1.9418045769
C 5.357195299 -0.8054709345 -1.805810202
H 6.0171422168 -0.7888867134 -2.6677740685
C 5.7966812206 -1.2627055952 -0.5730424286
H 6.8212317236 -1.5989308775 -0.4410955891
N -0.8497888058 -1.2885940275 -3.3823372617
H -1.4626885094 -1.7397793823 -4.0485040366
N 3.6461901065 0.0366422533 -3.2048726819
H 4.4330965844 0.2977367166 -3.7820729093
H 3.2420804531 -1.0552499403 2.226017155
N 2.7458105824 -0.7686532352 1.390874105
N -1.2386237058 1.520524041 0.4521098776
H -1.481334466 2.4575575821 0.1438394537
Co 1.0813320034 0.1769692465 -1.2645265761
C 1.2895160932 2.1921766926 -1.6746387477
O 2.4701805226 2.4387287866 -1.9621859631
O 0.2475652341 2.8607400286 -1.5795628141

```

Listing S66. Coordinates of the transition state for forming one intramolecular hydrogen bond in complex **1^(I)**-CO₂. (Corresponds to the structure labeled “TS 1” in Figure S49.)

```

H 2.4700745708 0.2109263942 3.796335426
C 1.7120378995 0.5762504548 3.1083580358
C 0.5879362662 1.237602551 3.5713524866
H 0.4459925453 1.3985504189 4.6364750717
C -0.3545786563 1.6935385142 2.645736177
H -1.2553454713 2.2180550924 2.9409236302
C -0.1227060489 1.4709935477 1.2938622603
N 0.987998846 0.845428607 0.8146533609
C 1.8772587211 0.3952796438 1.71917128
C -1.6560440682 0.8590624825 -0.4083634619
C -2.9299234328 0.4067416646 -0.0806578578
H -3.4564469135 0.8765265898 0.7415975029
C -3.4967129853 -0.6159035519 -0.8458073255
H -4.4897319682 -0.9949863666 -0.6204319182
C -2.7833016986 -1.1218215325 -1.9195815218
H -3.2022530541 -1.8975408605 -2.5554981806
C -1.5029191534 -0.5996708386 -2.194490414
N -0.9179050832 0.3405447612 -1.4290925967
N 1.3265069046 -0.1529242772 -3.3077912255
C 0.3482545893 -0.818192524 -3.9494712487
C 0.4885830638 -1.2978237282 -5.2685424449
H -0.3396698254 -1.8118466297 -5.7492851879
C 1.6814597311 -1.0860022449 -5.9375730556
H 1.8075669636 -1.4361987893 -6.9583631249
C 2.7141095248 -0.4144580137 -5.2776420232
H 3.6719773343 -0.21620937 -5.7432631513
C 2.5003408323 0.0217459746 -3.975753485
H 5.1711407188 -1.714264899 1.0737141275
C 4.8518340829 -1.2470517219 0.1456327808
C 3.6768094969 -0.468642004 0.1157739698
N 3.2131817997 0.1113189914 -1.0070361892
C 3.9833202343 0.0045884634 -2.1256655335
C 5.1608367904 -0.7341966493 -2.1741553777
H 5.7220455388 -0.7639273727 -3.1005506412
C 5.5935354871 -1.3848534904 -1.0157610752
H 6.5084350149 -1.9709605447 -1.0151934895
N -0.8556918561 -1.1070156832 -3.3158186772
H -1.4433116244 -1.7247561417 -3.8584647078
N 3.5503246489 0.6915669491 -3.2881166075
N 3.0022420298 -0.3198938817 1.3227267561
N -1.0837384837 1.9160928042 0.3438372668
Co 1.1853617543 0.6955092095 -1.3279463003
H 3.5091915905 -0.7131901066 2.1035431771
H -0.6023310894 2.5783219741 -0.3132436488
H 3.1976103942 1.6407003776 -3.0102161377
C 1.3431738633 2.6655219275 -1.792830701
O 2.335653343 2.9682284945 -2.4904478813
O 0.4326768324 3.3916353342 -1.337888118

```

Listing S67. Coordinates of $1^{(n)}$ -CO₂ forming two intramolecular hydrogen bonds. (Corresponds to the structure labeled “2 H-bonds” in Figure S49.)


```

H 2.3628506495 0.3319508719 3.7683115133
C 1.6462714032 0.6841159033 3.0308141678
C 0.549977209 1.4432426412 3.4074086914
H 0.3904420655 1.694343309 4.4523551041
C -0.3411049672 1.8788700413 2.4220168486
H -1.2189592348 2.4713064216 2.6508564063
C -0.0889427837 1.5362072469 1.1001046162
N 0.9960201432 0.8141017603 0.7067434879
C 1.8366515742 0.3899583434 1.6660118848
C -1.5948183844 0.7853340705 -0.5402563165
C -2.8537778895 0.3487277775 -0.1376372046
H -3.3795055774 0.8960261806 0.6359602189
C -3.4048949947 -0.7695742887 -0.768675809
H -4.3835473625 -1.1428798853 -0.4791511776
C -2.7034794603 -1.3794099003 -1.7990724429
H -3.1163368368 -2.2284472811 -2.3374934989
C -1.4467928904 -0.8588429993 -2.1583339415
N -0.8671827688 0.1626988271 -1.5032061963
N 1.384793173 -0.4942424807 -3.2939130645
C 0.2892268216 -0.8954109512 -3.9732856942
C 0.1889414754 -0.8397682276 -5.3652746741
H -0.7305350524 -1.1349522622 -5.8619367446
C 1.2815314911 -0.3592639707 -6.0892621422
H 1.2308590938 -0.2848054324 -7.1720442297
C 2.4385853656 -0.005808496 -5.4133737431
H 3.333836562 0.3140389537 -5.9354862861
C 2.4619074574 -0.1230940568 -4.0126881392
H 5.3134264281 -1.3895016235 1.3581529685
C 4.9774820089 -1.1113972864 0.362545969
C 3.6930941781 -0.5615022194 0.1841615991
N 3.2054305417 -0.1926720679 -1.0195556853
C 4.0443769568 -0.3285244199 -2.0830792499
C 5.3255110266 -0.8658694199 -1.9866775132
H 5.9200803561 -0.9634183338 -2.8874697071
C 5.8023219107 -1.2676061574 -0.7374813537
H 6.797481374 -1.6888127351 -0.6282080587
N -0.7859708526 -1.4314742806 -3.2454355139
H -1.3947175984 -2.0056157451 -3.8136441201
N 3.671631064 0.1297169807 -3.3702173298
N 2.9274229607 -0.4144830292 1.3403840646
N -1.0074879164 1.9193197075 0.0802259315
Co 1.2751130424 0.4289611721 -1.3479290906
H 3.4231793604 -0.7306199109 2.1627132881
H -0.4762994848 2.4622005581 -0.6412825926
H 4.0003546861 1.0797336246 -3.537467305
C 1.6396817472 2.3578879954 -1.9525292037
O 2.7474097901 2.5628677163 -2.4729687601
O 0.665192139 3.1152773581 -1.7338499714

```

Listing S68. Coordinates of the transition state for forming the second intramolecular hydrogen bond in complex **1^(I)-CO₂**. (Corresponds to the structure labeled “TS 2” in Figure S49.)

H	2.38358	-0.43654	3.66332
C	1.73060	0.06001	2.98355
C	0.73973	0.96546	3.45243
H	0.63041	1.12769	4.50889
C	-0.07194	1.60189	2.53326
H	-0.86576	2.26339	2.83094
C	0.09530	1.31646	1.16282
N	1.04729	0.46396	0.70486
C	1.83246	-0.12164	1.59032
C	-1.50297	1.02182	-0.62335
C	-2.90983	1.09422	-0.66677
H	-3.40626	1.82871	-0.05304
C	-3.60433	0.18323	-1.42831
H	-4.67831	0.17874	-1.46989
C	-2.87668	-0.79749	-2.16911
H	-3.38117	-1.50592	-2.77836
C	-1.47013	-0.75152	-2.08219
N	-0.79799	0.10310	-1.33854
N	1.30895	-0.54447	-3.10820
C	0.32654	-1.27327	-3.67211
C	0.32029	-1.64051	-5.01972
H	-0.50587	-2.21466	-5.42494
C	1.36628	-1.20712	-5.82879
H	1.38095	-1.45654	-6.88751
C	2.39036	-0.45955	-5.27092
H	3.23673	-0.12940	-5.86175
C	2.33618	-0.17008	-3.89889
H	5.47541	-1.06427	1.20535
C	5.08028	-0.72321	0.25429
C	3.69886	-0.61339	0.06915
N	3.13847	-0.17150	-1.07636
C	3.97250	0.14116	-2.09415
C	5.37134	0.09685	-1.97777
H	5.99287	0.36463	-2.82399
C	5.92196	-0.34314	-0.78492
H	7.00209	-0.39865	-0.66508
N	-0.74590	-1.68039	-2.85421
N	3.41342	0.49453	-3.31556
H	4.08071	0.84661	-3.98455
N	2.84514	-0.97710	1.12201
N	-0.81217	1.87934	0.24916
H	-0.79422	2.84668	0.08350
Co	1.18986	0.15492	-1.25530
H	3.34440	-1.43907	1.87163
C	1.32890	2.11991	-1.91216
O	0.99696	2.53341	-3.01787
O	1.83476	3.05493	-1.00950
H	1.85553	3.92380	-1.48595

Listing S69. Coordinates of the transition state for forming the singly hydrogen-bonded intermediate in complex **1^(II)-CO₂H**. (Corresponds to the structure labeled “TS 1” in Figure S51.)

```

H 2.2320009402 -0.5642570636 3.6600214694
C 1.5964889441 -0.0118384487 2.9744655196
C 0.58718072 0.815601505 3.439827171
H 0.4086098877 0.9177262249 4.5060119603
C -0.1841280069 1.5228136031 2.5149345271
H -0.9830102011 2.1902570267 2.8140448316
C 0.0695959665 1.3538275595 1.1614113561
N 1.0528134021 0.539938875 0.6875506751
C 1.8130316551 -0.107225346 1.5915314991
C -1.4828838531 1.0909180826 -0.593803842
C -2.869404963 1.089112824 -0.5378842539
H -3.3646949855 1.8310692862 0.0764629873
C -3.5741970506 0.1210580488 -1.2572194489
H -4.6591523872 0.088249959 -1.2278234145
C -2.865826798 -0.7946034375 -2.0187809046
H -3.3760740682 -1.551719266 -2.6064452137
C -1.4656664016 -0.7125414288 -2.051633279
N -0.7729989739 0.1956403963 -1.3372740745
N 1.3225974947 -0.52383232 -3.1139032895
C 0.3156196818 -1.2309559478 -3.6728101273
C 0.2934310529 -1.5978677658 -5.0185230883
H -0.5497808493 -2.1514203145 -5.4183358876
C 1.3446814308 -1.1925285401 -5.8370007398
H 1.3455417734 -1.4407634981 -6.8938903072
C 2.3930080082 -0.4753619157 -5.2829246244
H 3.2453172293 -0.1692149647 -5.8804253084
C 2.358463676 -0.184495784 -3.9133648583
H 5.4750187709 -1.0091344261 1.23469531
C 5.0878704118 -0.6877545818 0.2734329466
C 3.7100060834 -0.5715665107 0.0780517754
N 3.1579370278 -0.1474442844 -1.0826776052
C 4.0056364584 0.1209064441 -2.1055058216
C 5.4000476891 0.0705348714 -1.9764472859
H 6.0305676957 0.3072703702 -2.8271746462
C 5.9424086205 -0.3389440149 -0.7679517614
H 7.0188214863 -0.3974979185 -0.6390698264
N -0.7521171108 -1.6124140772 -2.8479798912
N 3.4643877819 0.4286716531 -3.3408588991
H 4.1356822799 0.7729611317 -4.0150418184
N 2.8539602693 -0.914490602 1.1292512441
N -0.7657470606 2.012424924 0.2180764476
H -0.2029094136 2.6730252417 -0.3325090659
Co 1.2152647078 0.2234739032 -1.2776981839
H 3.3421936667 -1.3832832026 1.8826661202
C 1.4028796485 2.1705661638 -2.029149104
O 1.3671102773 2.5171094436 -3.1985934932
O 1.5359538116 3.2047795781 -1.0780970599
H 1.6083016441 4.0488128232 -1.576723624

```

Listing S70. Coordinates of the singly hydrogen-bonded intermediate in complex **1^(II)**-CO₂H. (Corresponds to the structure labeled “1 H-bond” in Figure S51.)

```

H 2.2741651629 -0.6143716613 3.6570701795
C 1.6211827208 -0.0583452542 2.9911392436
C 0.6113857157 0.7500472852 3.4855895196
H 0.4477407591 0.8345018790 4.5557635455
C -0.1853066929 1.4543246198 2.5815882070
H -0.9960127028 2.0977930845 2.9004973375
C 0.0467146267 1.3093139303 1.2199238879
N 1.0431856317 0.5259108806 0.7163531255
C 1.8185173297 -0.1287863766 1.6034536456
C -1.5237885575 1.0535849851 -0.5260662737
C -2.9104932051 1.0191510245 -0.4549509325
H -3.4098618364 1.7198148753 0.2028643820
C -3.6063120815 0.0714255885 -1.2064332029
H -4.6898766671 0.0135029752 -1.1653159465
C -2.8861219982 -0.7963974924 -2.0102973853
H -3.3850749625 -1.5432269007 -2.6204679314
C -1.4882895410 -0.6817993525 -2.0557134973
N -0.7998824411 0.2178915014 -1.3247543726
N 1.3160394019 -0.4915677471 -3.1405398048
C 0.2874648637 -1.1664270391 -3.7068282534
C 0.2433301784 -1.5137396799 -5.0573336675
H -0.6225545294 -2.0310812948 -5.4570150405
C 1.3024299509 -1.1368455037 -5.8796079428
H 1.2850896490 -1.3660787034 -6.9406646206
C 2.3856987815 -0.4841948746 -5.3185443164
H 3.2564354101 -0.2218521114 -5.9102237291
C 2.3765747562 -0.2200659056 -3.9393274622
H 5.4738642033 -0.9272996626 1.2700574848
C 5.0945383373 -0.6302330868 0.2979703120
C 3.7190925925 -0.5513331864 0.0796301671
N 3.1688420902 -0.1547874386 -1.0933273252
C 4.0271168622 0.0876670998 -2.1143006317
C 5.4229906014 0.0887444558 -1.9586713932
H 6.0580703753 0.3186504543 -2.8077424689
C 5.9576591932 -0.2716439417 -0.7349237029
H 7.0329837379 -0.2923446792 -0.5867957686
N -0.7818885281 -1.5488114478 -2.8898019965
N 3.5310841439 0.2785886367 -3.3821467509
H 4.1862875100 0.6756608569 -4.0418003769
N 2.8622296124 -0.9187726199 1.1230618622
N -0.8318851160 1.9574140722 0.3172664983
H -0.3446760587 2.6847343382 -0.2311979332
Co 1.2152711080 0.2740082802 -1.2804070930
H 3.3588532614 -1.3894775002 1.8697410485
C 1.5590232067 2.2805972355 -1.9304225307
O 2.3906400415 2.6550436416 -2.7428034444
O 0.7679207139 3.3231905299 -1.3930408099
H 1.0681141868 4.1644266992 -1.8026137749

```

Listing S71. Coordinates of the barrier for intramolecular proton transfer in **1^(II)-CO₂H**.
(Corresponds to the structure labeled “TS 2” in Figure S51.)

```

H 2.1950781138 -0.6996764063 3.6430549847
C 1.5879650204 -0.1073370149 2.9650202028
C 0.5659617916 0.7002867429 3.4356664831
H 0.347650975 0.745191725 4.4983989594
C -0.1668146938 1.4691624656 2.5265375381
H -0.9719605093 2.1270888296 2.8353698695
C 0.142508835 1.3669590371 1.1791956666
N 1.1227442456 0.5580969225 0.6920415646
C 1.8518023464 -0.1352286162 1.5863375109
C -1.4083897299 1.1634212823 -0.5620911787
C -2.7886159922 1.1522733463 -0.4309858896
H -3.2625873668 1.8824168633 0.2160728749
C -3.5152734252 0.1774300143 -1.1211456223
H -4.5969306902 0.1330551243 -1.0368864747
C -2.8380064577 -0.7257615766 -1.9233496284
H -3.369802563 -1.4844530871 -2.4896332955
C -1.4405351927 -0.6351798496 -2.0210315958
N -0.722169391 0.2726725354 -1.3324456227
N 1.3448679789 -0.5118608786 -3.1210322986
C 0.311241361 -1.1844111026 -3.6746754812
C 0.2701721105 -1.5522131466 -5.0199701792
H -0.5939112836 -2.0762028495 -5.4149895001
C 1.3314923173 -1.1864962657 -5.8436117172
H 1.3191599752 -1.4370211277 -6.899879116
C 2.4065601619 -0.5053431842 -5.2955040536
H 3.2662977276 -0.2300897717 -5.8973373041
C 2.3874401121 -0.2089206596 -3.9267956342
H 5.5169694127 -1.0365725333 1.221010859
C 5.1312751653 -0.7199312045 0.2576178515
C 3.7540243221 -0.5891906021 0.0654575688
N 3.2036084064 -0.1662205179 -1.0975755499
C 4.0524925007 0.0753149797 -2.1267466948
C 5.4466405933 0.0072698747 -2.0012974437
H 6.0772625088 0.2242677213 -2.8571833435
C 5.987367262 -0.3933210764 -0.7893826711
H 7.0632961025 -0.463702417 -0.6624983939
N -0.7636385193 -1.5333834532 -2.8473551247
N 3.5146913425 0.3733725615 -3.364836693
H 4.189601135 0.6983924285 -4.0448656619
N 2.9026487478 -0.923885568 1.1215632692
N -0.6377313232 2.0831710686 0.2177480953
H 0.0018870169 2.6368890718 -0.3689516042
Co 1.2714606456 0.2520286373 -1.2878013513
H 3.3866039544 -1.40662044 1.8686849326
C 1.5163084336 2.1867363157 -2.0630601424
O 1.5062780034 2.5276107556 -3.233771205
O 1.6596087817 3.2262078847 -1.1147340373
H 1.749249912 4.0670200531 -1.6160015092
O -2.5959085903 3.6082406113 1.7839830598
H -1.8623633102 3.4188960623 1.1644735335
H -2.7145036596 4.5697932278 1.8024389843

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Listing S72. Coordinates of the singly hydrogen-bonded intermediate in complex **1^(II)-CO₂H** in the presence of an explicit water molecule. (Corresponds to the structure in Figure S52.)

```

H 2.5615110986 -0.2793201881 3.7212599696
C 1.8502210986 0.1870298119 3.0499599696
C 0.8418610986 1.0054298119 3.4955399696
H 0.7075110986 1.1931398119 4.5578399696
C -0.0249289014 1.5950198119 2.5594299696
H -0.8589289014 2.2180498119 2.8669299696
C 0.1691710986 1.2950198119 1.2181799696
N 1.1704210986 0.5209998119 0.7414599696
C 2.0672310986 -0.0099901881 1.6508899696
C -1.4466089014 0.9453098119 -0.5667800304
C -2.8393089014 1.0604798119 -0.7036500304
H -3.3687789014 1.8494698119 -0.1793200304
C -3.5121289014 0.1220298119 -1.4683300304
H -4.5915389014 0.1734498119 -1.5791400304
C -2.7875389014 -0.8940801881 -2.0896100304
H -3.2761589014 -1.6375701881 -2.7112000304
C -1.3989989014 -0.9033301881 -1.9459700304
N -0.7231989014 -0.0035901881 -1.2036100304
N 1.3462810986 -0.6985501881 -3.0143700304
C 0.3692110986 -1.4801701881 -3.5117300304
C 0.3036310986 -1.8727901881 -4.8488500304
H -0.5173089014 -2.4915201881 -5.1970600304
C 1.2794010986 -1.3979401881 -5.7269700304
H 1.2444210986 -1.6631901881 -6.7798700304
C 2.2967510986 -0.5941501881 -5.2402100304
H 3.0950810986 -0.2327801881 -5.8798600304
C 2.3219110986 -0.2975401881 -3.8667700304
H 5.5841010986 -1.3480201881 1.0637299696
C 5.1768410986 -0.9775901881 0.1303899696
C 3.7974910986 -0.6119201881 0.1341699696
N 3.2065410986 -0.1752801881 -1.0344800304
C 3.9919510986 -0.0137701881 -2.1248300304
C 5.3574010986 -0.2631101881 -2.1495600304
H 5.9194110986 -0.1078101881 -3.0638100304
C 5.9529010986 -0.7753201881 -0.9862400304
H 7.0140110986 -1.0116601881 -0.9741000304
N -0.6436389014 -1.8814001881 -2.6181300304
H -1.2460289014 -2.5780401881 -3.0410100304
N 3.3700810986 0.3982198119 -3.3206000304
H 3.9921510986 0.8792798119 -3.9620800304
N 3.1891910986 -0.6615701881 1.3279299696
N -0.7661389014 1.7957498119 0.2835499696
H -1.3597389014 2.5125398119 0.6815399696
Co 1.2762910986 0.1218798119 -1.1821500304
H 1.9008210986 3.8371498119 -2.0939000304
C 1.1895710986 2.0484498119 -1.9994500304
O 2.2248610986 2.9900298119 -1.7144100304
O 0.2840610986 2.4902798119 -2.6952700304
O 4.5304710986 2.9804698119 -3.4534500304
C 5.5761653228 3.8065890118 -3.0047897236
H 3.7936510986 2.9474598119 -2.8015100304
C 5.4677163223 5.2110958268 -3.5911581496
F 5.4430184255 5.1987301396 -4.9420051049
F 6.5341341544 5.9676291360 -3.2115970937
F 4.3492056864 5.8528116338 -3.1746310579
H 6.5283105326 3.3823911767 -3.3432438159
H 5.6061746279 3.9031724827 -1.9129735341

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Listing S73. Coordinates of $\mathbf{1^{(II)}-CO_2H}$ in the presence of an explicit TFE molecule.
(Corresponds to the structure in the blue box of main text Figure 5.)

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